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In re Application of: Jonathan S. Brecher)
U.S. Serial No.: To Be Assigned)
Filed: Herewith (February 11, 2000))
(This application claims the benefit of U.S.)
Provisional Application Serial No. 60/119,930)
Filed on February 12, 1999))
Title: DERIVING CHEMICAL STRUCTURAL)
INFORMATION)

Box Patent Application
Assistant Commissioner for Patents
Washington, D.C. 20231

TRANSMITTAL LETTER

Dear Sir:

Enclosed herewith for filing in the above-referenced application are the following documents:

1. New U.S. Patent Application entitled **DERIVING CHEMICAL STRUCTURAL INFORMATION**
and naming as inventor(s): Jonathan S. Brecher
the Application including 50 pages comprising:
33 pages of specification including
2 pages of claims (claims 1-4) and;
1 page of abstract; and
17 pages of informal drawings (Figures 1 to 7G).
2. Declaration and Power of Attorney (unexecuted).
3. Appendix: NOMTOKENS and Cover Sheet for Appendix:NOMTOKENS.
4. Microfiche Appendix (382 frames on 4 sheets of microfiche).

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5. Postcard.

The Commissioner is hereby **not authorized** to charge the filing fees to our Deposit Account No. 08-0219.

Respectfully submitted,

HALE AND DORR LLP

Dated: February 11, 2000

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DERIVING CHEMICAL STRUCTURAL INFORMATION

CROSS-REFERENCE TO RELATED APPLICATIONS

This application claims the benefit of United States Provisional
5 Application Serial No. 60/119,930 entitled DERIVING A CHEMICAL
STRUCTURE FROM A CHEMICAL NAME filed on February 12, 1999,
incorporated herein.

REFERENCE TO MICROFICHE APPENDIX

10 A microfiche appendix forms part of this application. The appendix,
which includes a source code listing relating to an embodiment of the invention,
includes 382 frames on 4 sheets of microfiche.

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reserves all copyright rights whatsoever.

Background of the Invention

This application relates to deriving chemical structural information.

20 A chemical substance is commonly represented in textual form ("name")
or graphical form ("structure"), each of which has its own advantages. For
example, a name such as "benzene" is well-suited for use in a conversational or

written statement such as "The object was immersed in 100% benzene." Benzene can also be represented by a structure (Fig. 1) that illustrates that a benzene molecule features high symmetry, including six carbon atoms arranged at the corners of a regular hexagon, with six hydrogen atoms arranged a fixed distance outward from respective corners.

A chemical substance can have multiple chemical names. For example, benzene is also known as "benzol", "cyclohexatriene", "1,2,3-cyclohexatriene", "cyclohexa-1,2,3-triene", "[6]annulene", and "1-carbapyridine". Some names are sanctioned by at least one of three major organizations that have developed chemical nomenclature systems: the International Union of Pure and Applied Chemistry ("IUPAC"), the International Union of Biochemistry and Molecular Biology ("IUBMB"), and the Chemical Abstracts Service ("CAS"), a division of the American Chemical Society ("ACS"). These organizations often disagree about the preferred name for a substance, and the recommendations from each organization tend to be complex and have changed over time. In many instances, chemists produce or use chemically correct names that vary from the "sanctioned" names. Unintentional errors such as typographical errors are common.

Chemical names are commonly found in one of two general forms, known as "normal" (e.g., "O-acetylsalicylic acid") and "inverted" (e.g., "salicylic acid, O-acetyl-"). Each form has its utility. The normal form corresponds to

regular English writing style, is read from left to right, and is appropriate for use in prose. The inverted form emphasizes the main chemical feature of the substance and is particularly well suited for indexing, since the inverted form allows substances of similar chemistry to be sorted together, alphabetically.

5 Many chemical names are available only in inverted form.

The abundance of different names for the same chemical substance can create confusion and uncertainty when one chemist attempts to understand a written document produced by another chemist. Chemical structures, on the other hand, tend to cause less confusion and uncertainty.

Summary of the Invention

10 A method and a system are provided for deriving, from chemical names, corresponding structures with high accuracy and comprehensiveness. An implementation in a high speed computer allows chemical names to be
15 accurately converted to chemical structures in real time or nearly in real time, which provides users with a powerful, practical tool for use in situations where structural representations offer substantial advantages. In at least some cases, the method and the system are able to derive such structures where the names do not conform to any sanctioned nomenclature system. By grouping chemical
20 name fragments into a small number of classifications, the method and the system feature flexibility that facilitates application of the method and the system

to new chemical names as well as old chemical names, including names for organic and inorganic substances. The method and the system handle inverted names, including inverted names with missing commas or with extraneous spaces.

Other features and advantages will become apparent from the following description, including the drawings, and from the claims.

Brief Description of the Drawings

Fig. 1 is an illustration of a chemical structure.

Fig. 2 is a block diagram of computer-based systems.

Figs. 3A-3B and 4 are flow diagrams of computer-based procedures.

Figs. 5A-5D, and 6 are illustrations of computer data.

Figs. 7A-7G are illustrations of output produced by software.

Detailed Description

This application is filed simultaneously with a United States Patent Application entitled ENHANCING STRUCTURE DIAGRAM GENERATION, serial no. _____, which is incorporated herein.

Fig. 2 illustrates a structure derivation system 10. A chemical name 12 is supplied via one or more input systems such as end-user keyboard input 14, file-based input 16, or World-Wide Web query input 18. The chemical name is received by computer-based internal processing 20, which derives structural output in one or more forms such as a diagram 22 displayed on paper or on a

screen, a chemical format file 24, or a graphical format file 26. One or more of the output forms may be derived from another of the output forms, e.g., by scanning a paper printout into a computer file, or by using a graphic display program to display or print a diagram based on the contents of a format file.

5 In general, in a preferred embodiment, the internal processing operates by comparing portions of the chemical name to text strings that have been predetermined to have respective characteristics and properties in accordance with rules of chemical nomenclature, and with exceptions to such rules, and assembling a structure from pieces corresponding to selected text strings, as
10 described below.

Figs. 3A-3B illustrate a method 100 of the internal processing, which is applied in a specific example ("Phenacyl bromide, p-napthoxy") after the following description. The chemical name ("original input name") is preprocessed to standardize its formatting and to simplify subsequent operations
15 (step 1010). In an initial stage of the preprocessing, the individual characters of the name are manipulated as follows without reference to the chemical meaning implied by the characters. The name is converted to all lower-case characters. Common typographical errors, including errors that relate to inadvertent addition, deletion, or transposition of characters, are identified using substring
20 searches and are corrected. Uncommon characters of chemical significance are

spelled out using common characters, so that, for example, the character “μ” (“μ”) is changed to “mu”.

Also during the preprocessing, if the name or a portion of the name has been submitted in inverted form (e.g., “acetic acid, 2-hydroxy-”), the name or portion is converted to its uninverted form (e.g., “2-hydroxyacetic acid”) by a procedure 2000 (Fig. 4). A chemical name is uninverted by identifying name fragment boundaries and reordering the name fragments in accordance with a normal form. Commas are common delimiters of such name fragments, but other delimiters are found as well, and not all commas serve as boundaries. In the identification, false boundaries are determined from context and are discarded.

In the uninversion process, fragments are reordered after all fragments are identified, and context is observed. An inverted name of the form a/b/c/d/e may or may not uninvert to e/d/c/b/a; the name may become e/b/a/c/d or any of several other possibilities. The contents of each fragment are examined to determine the fragment’s proper position relative to preceding fragments.

The uninversion process includes the following steps (Fig. 4). The input name is analyzed to mark all potential name fragment boundaries (step 2010). In a specific embodiment, the mark used is an @ sign, which is rarely used in chemical names. In another embodiment, it may be advantageous to use a non-printing character such as control-A (ASCII value 1) that has effectively no chemical significance.

The name is scanned from left to right and is copied, possibly with changes as now described, into a new temporary buffer (step 2020). During scanning, open- and close-parentheses and other enclosing marks are counted, and depths of enclosing marks are monitored. With some exceptions, characters are copied to the new buffer unmodified. Commas that are not enclosed within any level of enclosing marks are not copied, but are instead converted to @ signs. For simplicity, any space characters or additional commas immediately following such a comma are treated as having no syntactic significance, and are not copied.

Hyphens are also examined during the scan. If a hyphen is immediately followed by a space character and is not immediately preceded by a comma or a plus (“+”) or slash (“/”) character, the hyphen is converted to an @ sign. Any space characters or additional commas immediately following such a hyphen are treated as having no syntactic significance, and are ignored. Such treatment addresses a common typographical error of omitting a comma, such as the comma that should be present before the final word in “benzoic acid, 2-chloro- oxime”.

An apostrophe that immediately precedes a digit is also assumed to represent the typographical omission of a comma, and is treated as if a comma were present. Thus, a comma is inserted between the two pertinent characters, unless the characters are not enclosed in any levels of enclosing marks such as parentheses, in which case an @ sign is inserted instead.

From this point, actions occur within the temporary buffer (step 2030) and do not to change the length of the buffer, which has the same length as the name in the buffer.

The buffer is scanned for the presence of a text string ("substring") "+@-", which, if found, is replaced by a substring "+,-".

The buffer is scanned for the presence of a substring "mer" followed by any character except "c". Since such a sequence, if present, indicates with high likelihood the presence of a polymer descriptor such as a monomer, dimer, or oligomer descriptor in the remainder of the string, any @ signs present in the remainder of the string, i.e., to the right of the "mer" substring, are converted to spaces. Determining whether the "mer" substring is followed by the character "c" is important to avoid misinterpreting mercury compounds as polymers, so that, for example, "acetic acid@mercury (ii)@hydrate" is not erroneously converted to "acetic acid@mercury (ii) hydrate".

The buffer is scanned for any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, that is immediately followed by any number (i.e., including zero) of the characters "]", ")", "}", or "h", in any order, but that is not preceded by the character "d". If such a sequence is found, any @ sign that immediately follows the sequence is converted to a comma, so that, for example, "1h@3h@5h@2@4@6-pyrimidinetriene" is properly converted to "1h,3h,5h,2,4,6-pyrimidinetriene".

If the final character of the buffer is a hyphen, and the last @ sign, if present, in the buffer is preceded immediately by a single one of the characters "]", ")", or "}", which is in turn preceded by any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, the last @ sign is converted to a comma.

The buffer is scanned for any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, followed immediately by a close parenthesis, followed immediately by any number of the characters "]", ")", or "}", followed immediately by an @ sign, followed immediately by any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", or "?". If such a sequence is found, the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "a", "b", "A", or "B". If such an @ sign is found where that preceding character is preceded by either of the characters "a" or "b", which is preceded by any of the characters "(", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?" or a comma or an apostrophe, the @ sign is converted to a comma. Accordingly, for example, "4aa@8ab-dihydronaphthalene" is properly converted to "4aa,8ab-dihydronaphthalene".

The buffer is scanned for an @ sign immediately preceding any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", or an apostrophe, where character precedes any single one of the characters ")", "]", "}", "e", "z", "r",

"s", "E", "Z", "R", or "S". If such an @ sign is found that is preceded by any single one of the characters "e", "z", "E", or "Z", which is preceded by any of the characters "(", "[", "{", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?" or a comma or an apostrophe, the @ sign is converted to a comma.

5 The buffer is scanned for an @ sign immediately preceding any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "a", "b", "A", "B", or an apostrophe, where such character itself precedes any single one of the characters "e", "z", "r", "s", "E", "Z", "R", or "S", or a period. If such an @ sign is found that is preceded by any number of the characters ")", "]", "}", or "*", which is preceded by any one of the characters "r", "s", "R", or "S", which is preceded by any of the characters "(", "[", "{", "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "a", "b", "A", "B", "?" or a comma or an apostrophe, the @ sign is converted to a comma.

 The buffer is scanned for any occurrences of the strings "@ar@" or ",ar@". Any such string that is found is converted to ",ar,".

15 The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) themselves precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "cis", "trans", "alpha", "beta", "gamma", "delta", or "epsilon". If such an @ sign is found that is preceded by any number of apostrophes or periods, which are preceded by any one of the strings "alpha", "beta", "gamma", "delta", "cis", or "trans", the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "ortho", "meta", or "para". If such an @ sign is found that is preceded by any number of apostrophes or periods, which are preceded by any one of the strings "ortho", "meta", or "para", the @ sign is converted to a comma.

The buffer is scanned for an @ sign immediately preceding any number of periods, where such periods (if any) precede either i) any single one of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", "?", "n", "o", "p", "s", "N", "O", "P", or "S"; or ii) any of the text strings "cis", "trans", "alpha", "beta", "gamma", "delta", or "epsilon". If such an @ sign is found that is preceded by any number of the characters "0", "1", "2", "3", "4", "5", "6", "7", "8", "9", or an apostrophe, which are preceded by any single one of the characters "n", "o", "p", "s", "N", "O", "P", or "S", which is preceded by either i) no characters at all or ii) any single one of the characters "(", "[", "{", "-", an apostrophe, a comma, or a space, the @ sign is converted to a comma.

The foregoing regarding buffer scanning is also described by the following text strings formatted in accordance with regular expression notation, as described in Friedl, Jeffrey E. and Oram, Andy, eds., Mastering Regular Expressions, O'Reilly & Associates, 1997.

```
s/(@.*mer[^c].*)@/$1,/gi
```

s/([[^]d][0-9\?\[\]\h]*)@/\$1,/gi

```
s/([0-9\?\7\))@([^\@]*-)/$1,$2/gi
```

s/([0-9\^?]\)\[?]\)*@([0-9\^?])/ \$1,\$2/gi

```
s/([\\(, 0-9\\'\\?][ab])@([0-9\\?ab])/ $1,$2/gi
```

```
s/([0-9,\(\)[ez])@([0-9\^?]*[ezrs\])/ $1,$2/gi
```

s/([0-9ab.\(\[\^\]\[rs][\^*\])*)@([0-9ab\^\?]*[rsez\.])/\$1,\$2/gi

s/([@,]ar@)/,ar,/gi

$$s/(\alpha|\beta|\gamma|\delta|\text{cis}|\text{trans})[\backslash.\text{?}^*/\backslash.([nops0-9\text{?}]|\text{cis}|\text{trans}|\alpha|\beta|\gamma|\delta|\epsilon|\text{it}|\epsilon)/\$1,\$2/\text{gi}$$

```
s/(ortho|meta|para)[\.\?|\.\*([nops0-9\?]|ortho|meta|para)/$1,$2/gi
```

```
s/(/[[:@_]\-\\]([[:nops]]{0,9}\?|\.\*([[:nops]]{0,9}\?|alpha|beta|gamma|delta|epsilon)/$1,$2/gi
```

All remaining @ signs are treated as true name fragment boundaries, so that the buffer is broken into fragments at the @ signs and is reassembled as follows (step 2040) in an output buffer created to store a final string.

The first fragment is added to the output buffer. Each name fragment subsequent to the first fragment is treated sequentially in one of the three following ways.

(1) A name fragment that terminates in a hyphen is prepended to the contents of the output buffer.

(2) A name fragment that does not end with one of the strings in Table 1 (Fig. 5A), that does not start with one of the strings in Table 2 (Fig. 5B), that does

not contain any of the strings in Table 3 (Fig. 5C), and that does not contain the string "mer" followed by a character other than "c", is prepended to the output buffer. The instant name fragment, when prepended, is separated from the rest of the buffer by a space character if the instant name fragment is the overall
5 second fragment to be identified and if the first fragment was one of the strings listed in Table 4 (Fig. 5D); otherwise the instant name fragment is separated from the rest of the buffer by a hyphen. (It is to be understood that Tables 1-4 are not necessarily exhaustive, and may be adapted as necessary.)

(3) In all other cases a name fragment is appended to the output buffer
10 with a space character therebetween.

At this point, the uninversion process is complete and makes available the final contents of the output buffer to serve as the uninverted name (step 2050).
Preprocessing is complete.

Once preprocessed, the name is divided into a series of fragments (Figs. 3A-3B, step 1020). In particular, the name is divided into the smallest number of
15 meaningful fragments of a maximum length. For example, "pentane" is not divided into three fragments "penta", "n", and "e", since the latter two fragments would not be meaningful, but rather is divided into two meaningful fragments "pent" and "ane". In a specific embodiment, a fragment is determined to be
20 meaningful ("recognized") if an exact match for the fragment is found in a dictionary of known text strings ("lexicon") that is maintained by the system.

Each known text string is associated in the lexicon with at least one data object known as a nomToken (Fig. 6). A nomToken includes the text of the known text string as its name and is described by Type and Subtype data members, which allow similar fragments to be grouped in accordance with two levels of similarity. Examples of NomTokens are identified in this application's Appendix: NomTokens which is submitted herewith and is incorporated herein, and in which NomTokens are provided in the following format:

name{ | synonym | synonym | ... } <space> type <space> subtype <space> data

(It is to be understood that the Appendix: NomTokens is not necessarily exhaustive, and may be amended as necessary.)

A text string may be present more than once in the lexicon if the text string is associated with multiple different nomTokens. For example, the text string "amide" is associated with a first nomToken of type kTypeAcid to be used with a name such as "propanamide" and is also associated with a second nomToken, of type kTypeAcidPart2, to be used with a name such as "propanic acid amide". Each nomToken also contains a repeat count and an indicator that indicates whether a repeat count of 1 originated explicitly with the designator "mono", and other optional type-specific information. In a specific embodiment, some of the fields of the nomToken are completed within the lexicon, and others are populated through further processing.

Four data objects within a nomToken record the nomToken's chemical

significance: a connection table, a locant map, an attach-in map, and an attach-out map. The connection table includes information that specifies which atoms are connected to which bonds and information regarding characteristics such as atom types, charges, and isotopy. The locant map associates names of individual atoms with respective specific locations in the connection table. For example, an atom named "2" in "2-hydroxy-propanoic acid" may be a specific one of the carbon atoms, and a "3" atom may be a different one of the carbon atoms. Multiple locants can refer to the same atom: "beta" may refer to the same atom as did "2" above.

The attach-in map functions similarly to the locant map and stores a list of atoms identified in the connection table that are considered to be awaiting attachment. Such a list is particularly useful when constructing structures of esters of acids. The attach-out map associates a specific bond order to an attachment. For example, after the phrase "oct-3-ylidene" is interpreted, an entry in the attach-out map indicates that the "3" atom in the "oct" group should have an attachment of order 2. For both the attach-in and attach-out maps, the actual construction of the attachments is performed later in the process.

An attach-in indicates an atom that, in at least some circumstances, preferentially has another fragment attached to it. For example, "acetate" has four atoms: two carbons and two oxygens. A proper interpretation of "methyl acetate" specifies that the methyl group is attached to a particular one of the

oxygen. For a portion of the processing period, between the time that "acetate" is handled and the time that "methyl" is attached to it, an attach-in exists on that particular one of the oxygens. Then, when it is time to add the "methyl" fragment, the position indicated by the attach-in is where the "methyl" fragment is attached to the acetate.

In an example involving an attach-out, a fragment "prop" is acquired, indicating a chain of three carbon atoms. There are two ways the fragment can be attached to another fragment: (1) connecting from the first carbon atom, which would cause the three carbons to extend from the other fragment much as a flag extends from a flagpole to flap in the wind, and (2) connecting from the second carbon atom, which produces in a Y-like structure. (Connecting from the third carbon atom is, in most cases, equivalent to connecting from the first carbon atom.) One way that an attach-out may be added to a structure is via the fragment "yl". When interpreting the fragment "propyl", an attach-out is created at the default atom, which is the first carbon atom in this particular case. A name such as "propylbenzene" is consistent with the three carbon atoms of the "propyl" group sticking out in a row from the benzene fragment. On the other hand, the positioning of the attach-out may be specified explicitly. For the fragment "prop-2-yl", the attach-out is attached to the central carbon atom. A name such as "prop-2-ylbenzene" specifies that the three carbon atoms from the "prop" group are attached to the benzene in the Y-like pattern.

A locant is a name for a specific atom. In the "prop-2-ylbenzene" example above, "2" is a name for the second atom in the "prop" three-carbon chain. In this particular case, the name happens to be neatly descriptive since "2" is used for the second atom, but such a situation cannot be assumed. Each atom may have zero locants, one locant, or multiple locants. For example, "prop-beta-yl" would be the same as "prop-2-yl"; the central atom actually has three locants that can be used interchangeably: "2", "b", and "beta". Additionally, the set of locants for a given nomToken may change (i.e., one or more may be added, and one or more may be removed as no longer valid) during the course of processing.

As the preprocessed name is parsed into fragments, a parallel list is derived from the nomTokens corresponding to each fragment (step 1030). If a fragment is represented by more than one nomToken, the nomToken having the highest-ranked type is chosen, at least initially. Punctuation characters including spaces and commas are interpreted as delimiting adjacent fragments, but are not preserved. Unrecognized fragments are converted into nomTokens of type kTypeUnknown and are included in the given order relative to the recognized nomTokens. The parallel list also stores, for each nomToken, an identification of the type of character that immediately preceded the fragment in the preprocessed name: an open parenthesis, bracket, brace, or the start of the name; a space character; or another type of character.

The recognition of parentheses and other enclosing marks, if any, is

integral to the name fragmentation process. During the fragmentation, the phrase surrounded by the innermost pair of enclosing marks is parsed as a unit, and is then consolidated as a unit according to a consolidation process described below with respect to the full name. Accordingly, each group within a set of enclosing marks is treated as a single unit, which is consistent with the syntactic meaning of enclosing marks. All levels of enclosing marks are handled in the same way, recursively.

When complete, the list of nomTokens is examined sequentially to determine whether any series of $2...n$ adjacent nomToken names could be concatenated into a larger "buildable" nomToken (step 1040). This is due at least in part to the fact that a small number of chemical terms are commonly expressed with included punctuation, which the fragmentation process uses to divide the input name. For example, the phrase "mg/ml" could be interpreted as possibly unrecognized nomTokens "mg" and "ml". Accordingly, "mgml" is recognized as a nomToken of type kTypeBuildable, which allows the two nomTokens "mg" and "ml" to be combined into one nomToken. The resulting nomToken of type kTypeBuildable is then converted to a nomToken of identical name and next-highest rank. For example, a fragment "xxxx" may be associated with three nomTokens, all named "xxxx", with respective values of 73, 42, and 21. The fragment may start off with the nomToken of value 73 and then may be converted to the "next-highest rank" nomToken, of value 42, and may

subsequently be converted to the next "next-highest rank" nomToken, of value 21.

The list of nomTokens is searched for a nomToken of type kTypeStopword, examples of which are identified in the Appendix: NomTokens (step 1050). If such a nomToken is found, the found nomToken and all subsequent nomTokens are removed from the list and are discarded (step 1060). This is due at least in part to the fact that chemical names are commonly found with additional descriptive text immediately following (e.g., "acetic acid" followed by "99% solution"), where the descriptive text does not contribute any information regarding the chemical structure of the chemical substance. The descriptive text is recognized and removed so that the remainder (e.g., "acetic acid") can be analyzed effectively.

At the conclusion of the fragmentation process, the text string of the original input name has been successfully divided into one or more substrings, and a list of nomTokens has been constructed corresponding to a list of the substrings. The fragmentation process has focused primarily on information contained in the text itself (e.g., the sequence of characters and punctuation), not on the chemical significance of the resulting nomTokens.

A consolidation process derives, from a list of nomTokens, a smaller list that contains fewer nomTokens, e.g., one nomToken (step 1070). The consolidation process examines the environments of the nomTokens, i.e., the

types and subtypes of each nomToken and other nearby nomTokens, and then, in each case, joins two or more nomTokens into a single replacement nomToken, as described below.

The consolidation process may determine that one or more nomTokens are misidentified. For example, a nomToken of type kTypeNatDeriver serves only to modify another nomToken that refers to a natural product, i.e., a nomToken of type kTypeRoot and subtype kSubtypeNatural. NomTokens of kTypeRoot pertain to collections of atoms connected by collections of bonds in a predetermined pattern, and correspond roughly to "root" or "core" fragments of a molecule.

In the absence of a nomToken that refers to a natural product, the nomToken of type kTypeNatDeriver is determined to have been misidentified. In such a case, the nomToken of type kTypeNatDeriver is converted to an identically-named nomToken of next-highest-rank, if any. If no identically-named nomToken of lower rank is found, the nomToken is converted to a nomToken of type kTypeUnknown, which is the lowest possible rank.

One suitable system of ranking of types is described herein (see also Appendix: NomTokens and the source code appendix under "enum nomTokenType"), but there are other suitable systems of ranking as well. With any suitable system of ranking, all consolidation steps are to be considered in light of the characteristics of that system of ranking. In at least some cases, it is

important that nomTokens be considered and acted upon in a particular order, so that nomTokens of the necessary rank are available when needed, and have not already been examined and converted to other nomTokens of lower rank.

The consolidation process begins with environments that are most specific. For example, characteristically, nomTokens of type kTypeCrown are immediately preceded and immediately followed by numerals, which are represented by nomTokens of type kTypeUnknown, for fragments consisting entirely of numeric digits. If such environments are found, a connection table for a crown ether may be constructed, and all three nomTokens may be replaced by a single nomToken containing the connection table. A nomToken of type kTypeCrown that is not preceded and followed by numerals is determined to be misidentified and is, as described above, therefore converted into the next-highest-ranked nomToken and retained in the list for later processing.

Consolidation continues with a series of less-localized nomenclature types characterized as sometimes appearing in multiple non-adjacent fragments. For example, interpretation of atomic chains may be performed at this stage. A nomToken of type kTypePrefix, such as "pent" or "penta", may refer implicitly to an alkyl or heteroatomic chain. The "penta" in "pentadiene" necessarily refers to a five-carbon chain. In a suitable environment, when followed by a nomToken of kTypeYl, such as "yl", "penta" is identified as referring to an alkyl chain, an appropriate connection table is constructed, and the nomToken is converted to

kTypeRoot, which is described above. In a different environment, when followed by a nomToken of kTypeRoot, "penta" indicates that the root structure should be repeated, and its original designation as kTypePrefix is retained for later handling.

5 The following description is with respect to the example of "penta". A pentane structure is a string of 5 carbon atoms separated by single bonds, with a sufficient number of hydrogen atoms to make 4 attachments on each carbon: CH₃-CH₂-CH₂-CH₂-CH₃. This is an example of an atomic chain. Pentasilane is a similar structure with silicon atoms instead of carbon atoms:

10 SiH₃-SiH₂-SiH₂-SiH₂-SiH₃. This is an example of a heteroatomic chain. "Silane" is the single molecule SiH₄, where the central atom is connected to each of the four surrounding atoms by a single bond. However, "pentasilane" is not properly interpreted to mean arranging 5 individual silane molecules next to each other to produce SiH₄ SiH₄ SiH₄ SiH₄ SiH₄. On the other hand,

15 "hydroxide" refers to a single molecule OH⁻, where the negatively-charged oxygen is connected to the hydrogen by a single bond, and "pentahydroxide" is in fact properly interpreted to mean arranging 5 individual hydroxide molecules next to each other to produce OH⁻ OH⁻ OH⁻ OH⁻ OH⁻.

20 Cyclic systems are created and aromatic rings are fused at this point in the processing. As shown, the order of interpretation is important in the individual sections as well as in the interpretation process as a whole. A name such as

“benzocyclooctene” implies that chains (kTypePrefix, treated as described above) are to be interpreted first and then are to be closed (kTypeCyclo) before being submitted for participation in ring fusions (kTypeBenzo).

At this point, portions have been identified within the greater set of name fragments that correspond to structures known as “root” or “core” structures.

After the main root portions of the name are identified, the consolidation process continues with nomTokens that directly modify the main root portions. Such directly modifying nomTokens generally correspond to grammatical prefixes and suffixes within the original input name. In at least one embodiment, many nomTokens representing traditional chemical functional groups are recognized at this stage, including acids in variations, radical suffixes such as “-yl,” and prefixes of heterocyclic “aza” nomenclature. Since there are many text strings that correspond to multiple nomTokens for functional groups, it is advantageous to examine the environments carefully for details.

In the last stages of the consolidation process, multiple large groups are joined, so that typically, for example, ligands are joined to root structures, cations to anions, and esters to acids.

An attach-out map having at least one remaining entry is present at the end of the consolidation process for a name such as “methyl” that is usually intended to be joined to another name fragment. An appropriate radical is added to the connection table for such remaining entry in the attach-out map, wherein,

for example, "methyl" is a monoradical and "methylidene" is a diradical.

The consolidated list of nomTokens is examined for any remaining nomTokens of type kTypeUnknown having names that correspond to known stereochemical indicators (step 1080). Stereochemistry is considered at this point because stereochemistry may be determined by the entire contents of a connection table. If a suitable nomToken is found, the appropriate stereochemistry is added to the connection table, and the nomToken representing the stereochemical indicator is removed (step 1090).

As shown, each action following the fragmentation of the original input name has attempted to reduce the number of nomTokens in the resulting list. If the list has been reduced by this point to a single nomToken, the nomToken's connection table, if present, represents the structure corresponding to the original input name. In such a case, a representation of the structure (e.g., an image of the structure) is derived from the connection table and is presented to the user (step 1100). (See, e.g., the above-cited simultaneously filed application.) If more than one nomToken is present, or if the single nomToken lacks a connection table, it is determined that the original input name is uninterpretable and an appropriate error message is presented instead (step 1110).

An example using a specific chemical name is now described. A name "Phenacyl bromide, p-naphthoxy" is submitted for processing. The name is preprocessed, including being converted to all lowercase characters, resulting in

“phenacyl bromide, p-naphthoxy”. A common typographical error “naph” is converted to “naphth”, which produces “phenacyl bromide, p-naphthoxy”. The name is uninverted, leaving “p-naphthoxy-phenacyl bromide”.

The name is divided into six recognized fragments and a list of six
5 corresponding nomTokens is created. These six nomTokens, with their types, subtypes, previous characters, and a graphical depiction of their connection tables, are shown in Fig. 7A.

The list of nomTokens is examined for recognized environments. The first
10 recognized environment is found when the list is examined for amino acids. No amino acids are found in the list, but one nomToken (“yl”) of type kTypeEnderAminoAcid is present. Such a nomToken, being meaningful only in the context of amino acids, is not meaningful in this list that contains no amino acids. Accordingly, the nomToken of type kTypeEnderAminoAcid is converted to the next-highest-ranked nomToken of identical name, which in this case is of
15 type kTypeSuffix and subtype kSubtypeYl (see Fig. 7B).

The next recognized environment is found in preparing to create
ortho/peri fused ring systems. One example of such an environment requires, among other things, adjacent tokens of types kTypeOPFuser and kTypeRoot. In this list of nomTokens, a nomToken of type kTypeOPFuser exists but is followed
20 by a nomToken of type kTypeInfix instead. Therefore, the nomToken of type kTypeOPFuser is determined not to be meaningful in this context, and is

converted to the next-highest-ranked nomToken of the same name, which in this case is of type kTypeRoot and subtype kSubtypeUnknown (see Fig. 7C).

The list is examined for nomTokens of type kTypeSuffix. Such a nomToken ("yl") is found, and is found to be preceded by a nomToken of type kTypeRoot, which results in a recognized environment. With respect to this recognized environment, an entry is added to the attach-out map of the root structure. In the absence of an explicit locant, the attach-out is assigned to the first atom in the connection table that has sufficient valences, which in this case is the terminal carbon (see Fig. 7D in which the attach-out is represented by a black diamond). The nomToken of kTypeSuffix is removed from the list, leaving five nomTokens in the list.

One of the nomTokens remaining in the list ("bromide") had been preceded by a space character in the preprocessed name. The space character may be chemically significant and is processed at this point. The list is divided into two smaller sublists, one of which contains the four nomTokens before the "bromide" nomToken, and the other of which contains the "bromide" nomToken only.

The first of the sublists is examined for nomTokens of type kTypeInfix. In this case, one nomToken of this type, "oxy", is found, and is preceded by another nomToken of type kTypeRoot, which results in a recognized environment. In this environment, the entire contents of the connection table of the kTypeInfix

nomToken are merged into the connection table of the root. Additionally, a bond is created between the first atoms with sufficient free valences originating in the two connection tables. Any entries (one in this case) in the attach-in and attach-out maps of the nomToken of type kTypeInfix are copied to corresponding atoms in the merged connection table. The subtype of the root structure is changed to kSubtypeInfix. The nomToken of type kTypeInfix is then discarded. The second of the sublists is similarly examined, but no changes are necessary in this case. At this point, the entire list has four nomTokens (see Fig. 7E).

In this example, only one other environment is recognized in the sublists, and is found in the first sublist. The first sublist contains a nomToken of kTypeRoot ("phenacyl") that is preceded by another nomToken of kTypeRoot ("naphthoxy") that has exactly one entry in its attach-out list. Furthermore, the further preceding nomToken is of type kTypeUnknown and has a name ("p") that corresponds exactly to one of the entries in the locant map of "phenacyl". Therefore, the connection tables for "naphthoxy" and for "phenacyl" are combined, and a bond is indicated between the atom referenced in the attach-out map of "naphthoxy" and the atom referenced by the "p" entry in the locant map for "phenacyl". Accordingly, with respect to the three nomTokens involved, two are discarded and the resulting connection table is stored in the third, which leaves two nomTokens in the entire list (Fig. 7F), with exactly one nomToken in each sublist. As no other environments are recognized in either sublist, the two

sublists are recombined.

The last environment that is recognized consists of a nomToken of type kTypeCounterion following a nomToken of type kTypeRoot, each of which nomToken has at least one entry in its respective attach-out list. In this
5 environment, the two connection tables are merged, and a bond is indicated between the two atoms referenced by the attach-out lists (Fig. 7G).

At this point, the list has a single nomToken, which is of type kTypeRoot and has a non-empty connection table. As the attach-out list has no entries, no radicals need to be added to the connection table. The name has been fully
10 parsed. The structure shown in Fig. 7G is the correct structure for the original name "phenacyl bromide, p-napthoxy", and is presented to the user.

All or a portion of the procedures described above may be implemented in hardware or software, or a combination of both. In at least some cases, it is advantageous if the technique is implemented in computer programs executing
15 on one or more programmable computers, such as a personal computer running or able to run an operating system such as UNIX, Linux, Microsoft Windows 95, 98, 2000, or NT, or MacOS, that each include a processor, a storage medium readable by the processor (including volatile and non-volatile memory and/or storage elements), at least one input device such as a keyboard, and at least one
20 output device. Program code is applied to data entered using the input device to perform the technique described above and to generate output information. The

output information is applied to one or more output devices such as a display screen of the computer.

In at least some cases, it is advantageous if each program is implemented in a high level procedural or object-oriented programming language such as Perl, C, C++, or Java to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

In at least some cases, it is advantageous if each such computer program is stored on a storage medium or device, such as ROM or optical or magnetic disc, that is readable by a general or special purpose programmable computer for configuring and operating the computer when the storage medium or device is read by the computer to perform the procedures described in this document. The system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner.

Other embodiments are within the scope of the following claims. For example, the system may be combined with one or more external databases of names and structures, so that a chemical name present in the external databases but not otherwise parsable would still produce a structure. In another example, non-English chemical names could be interpreted as well or instead. In another

example, the fragmentation of the initial chemical name may be varied, e.g., by using different or extended lists of known chemical name fragments.

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What is claimed is:

Claims

1. A method for use in deriving chemical structural information, comprising:

parsing a chemical name into at least first and second fragments; and

determining, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second diagrammatic representations of the first and second fragments.
2. The method of claim 1, further comprising:

identifying, among a preselected set of text strings, respective first and second text strings that correspond to the first and second fragments; and

basing the determination of the first and second diagrammatic representations at least in part on conditions associated with the first and second text strings.
3. A system for use in deriving chemical structural information, comprising:

a parser parsing a chemical name into at least first and second fragments;

and

a determiner determining, based at least in part on the positions of the

4. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive chemical structural information, the instructions causing the system to:

determine, based at least in part on the positions of the first and second fragments within the chemical name, respective first and second diagrammatic representations of the first and second fragments.

1991 1000

1991 1000

1991 1000

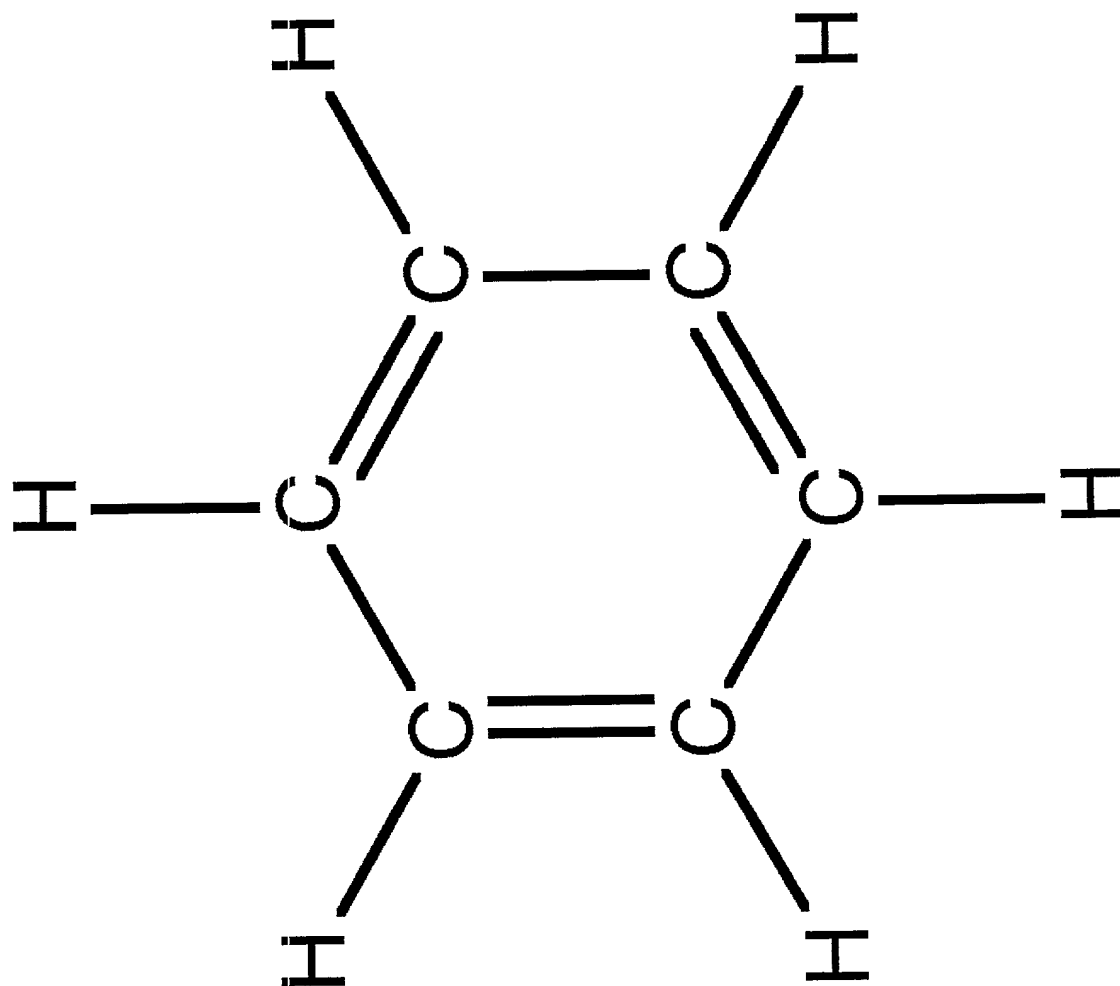
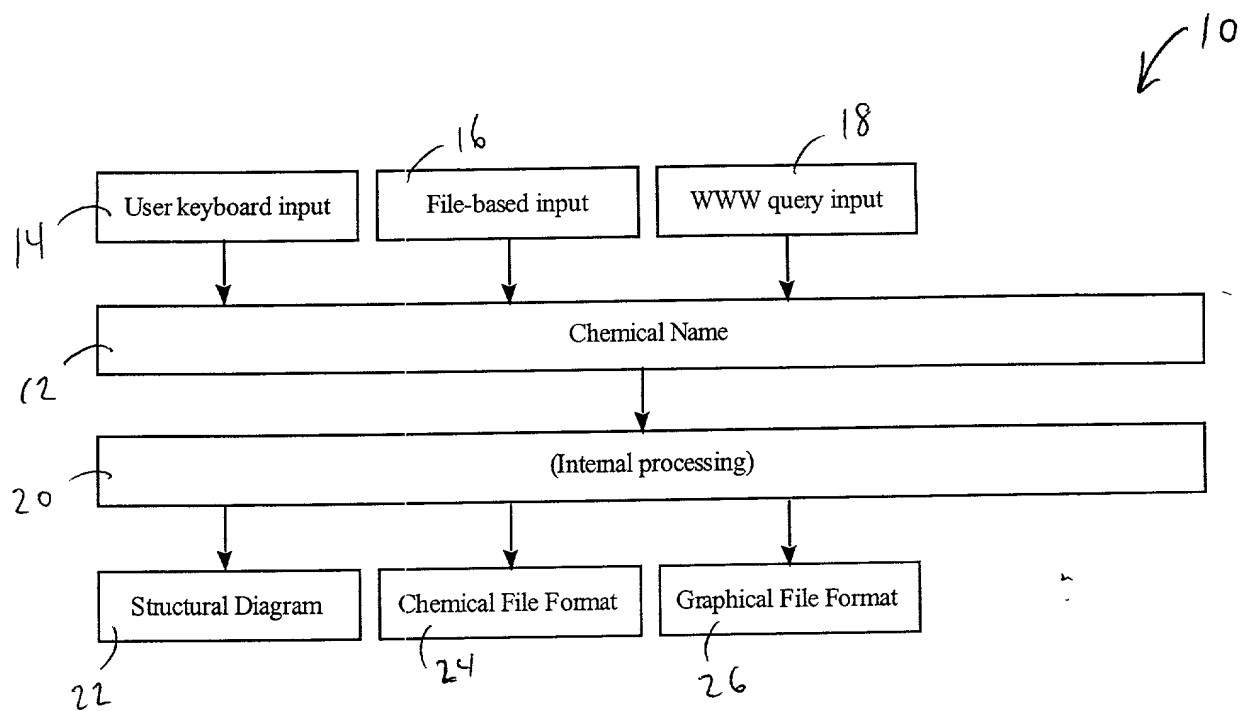


FIG. 1 (PRIOR ART)



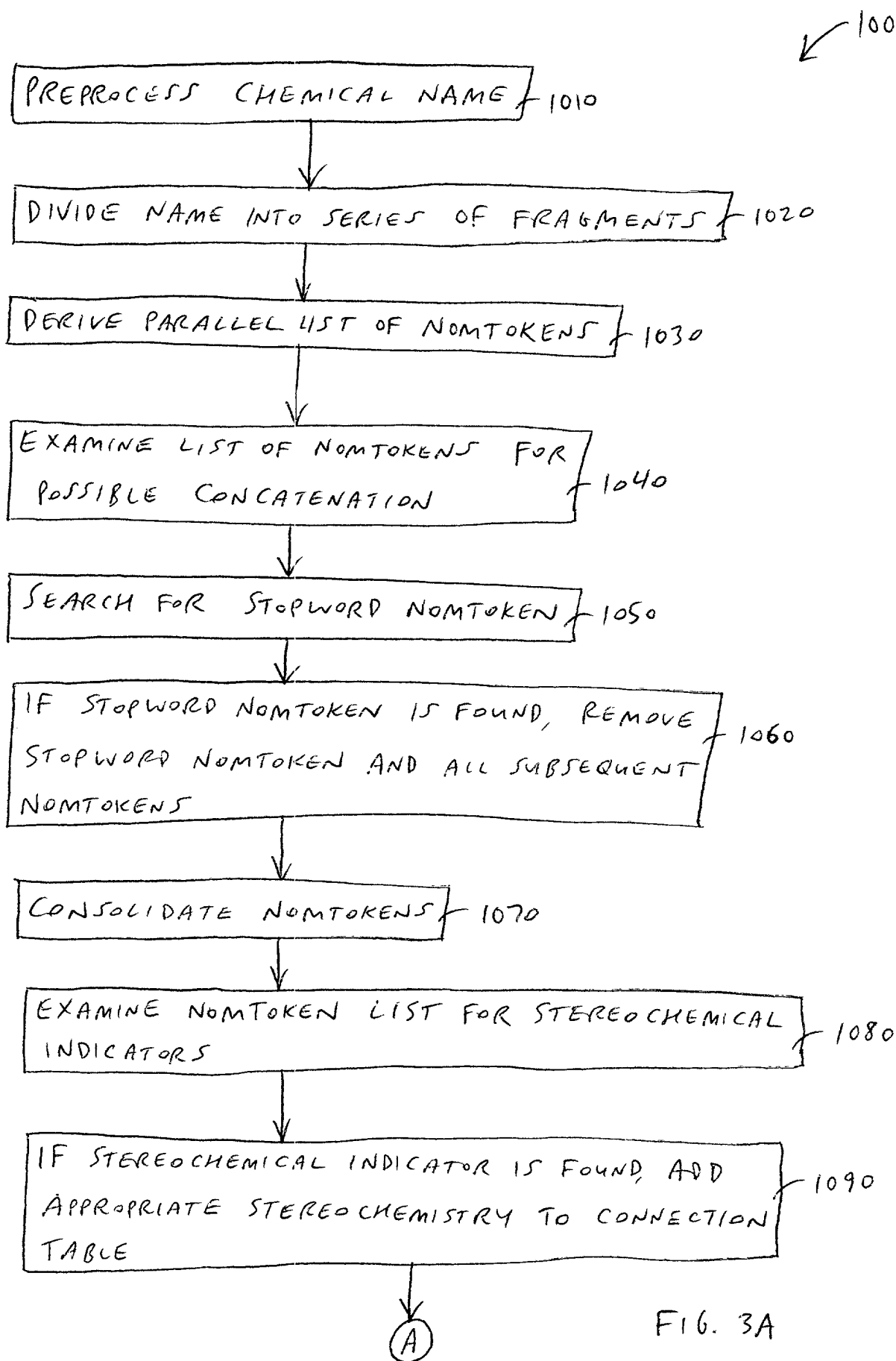


FIG. 3A

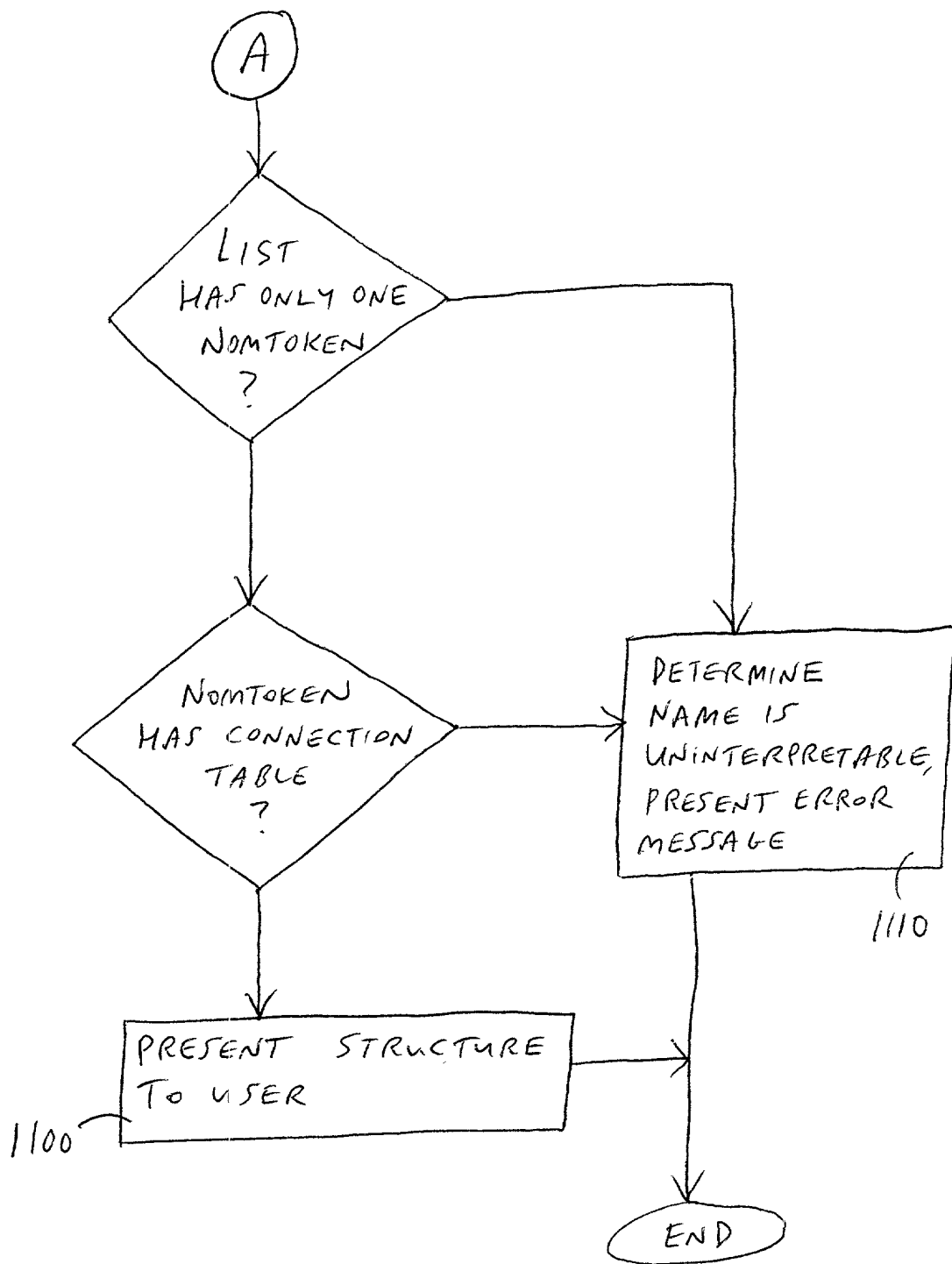


FIG. 3B

2000
↙

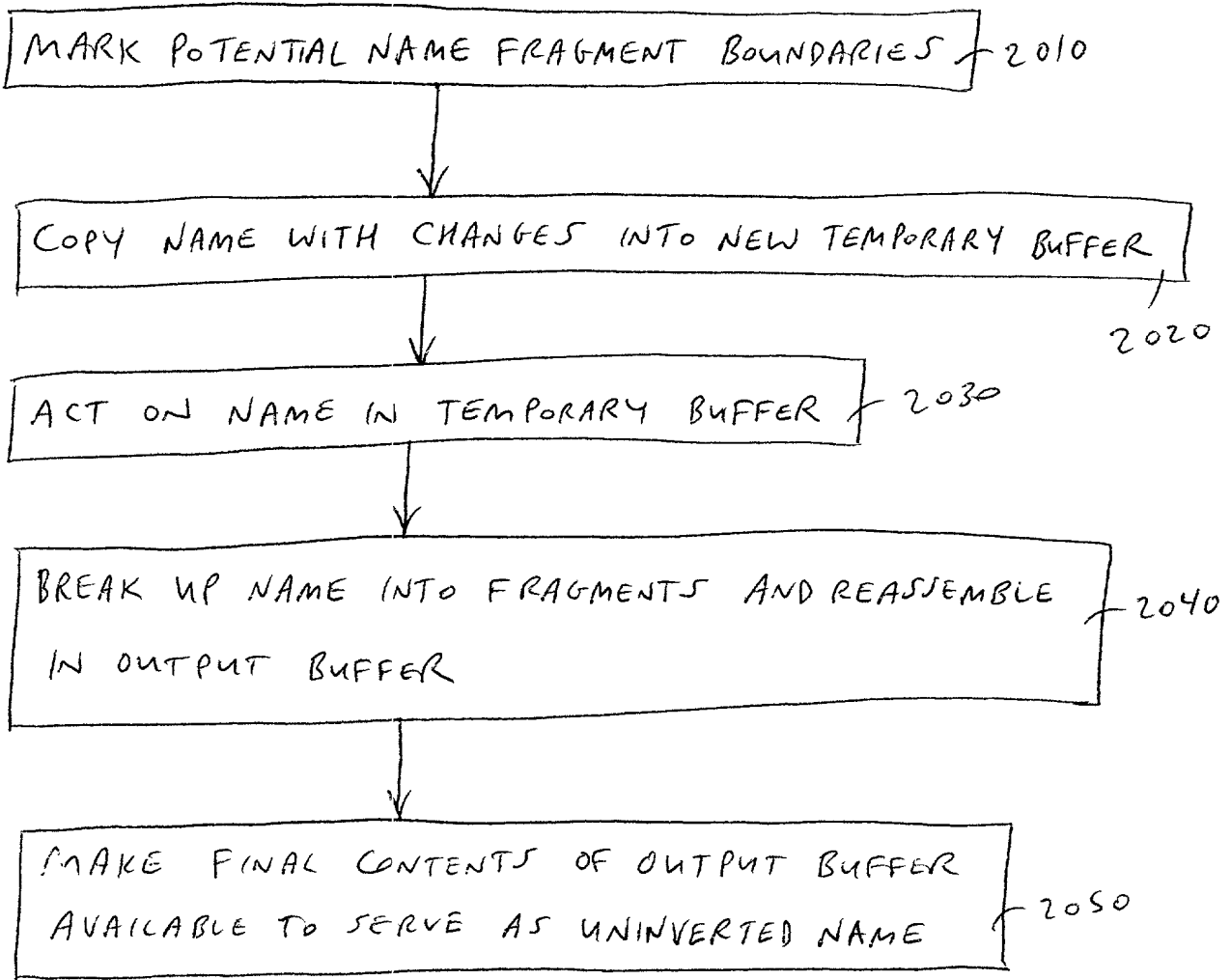


FIG. 4

Table 3: Strings that cannot appear anywhere in fragments to be prepended (note that some strings include one or more space characters)

" and "	"grade"	"radical"
" in "	"granul"	"random"
" ion"	"grease"	"reagent"
"&"	"grit"	"reduc"
" /"	"hbr"	"regular"
"7ci"	"hcl"	"remainder"
"8ci"	"heavy"	"ribbon"
"9ci"	"hydrin"	"rods"
"10ci"	"hydrous"	"salt"
"aas"	"ide "	"scale"
"absolute"	"imine"	"shot"
"acid"	"ing"	"slug"
"acs"	"inhibit"	"soluble"
"aerosol"	"isotop"	"solution"
"amidine"	"ite"	"sphere"
"analy"	"ize"	"spong"
"approx"	"lactam"	"stab"
"assay"	"lacton"	"stabil"
"ate"	"light"	"standard"
"balance"	"lump"	"stick"
"basic"	"mainly"	"sublim"
"basis"	"medium"	"sultam"
"bead"	"mesh"	"sulton"
"briquette"	"micron"	"synthetic"
"catal"	"ml "	"syrup"
"certif"	"mm "	"tablet"
"chip"	"moist"	"tech"
"chunk"	"morphous"	"tion"
"cm"	"mossy"	"titrant"
"coarse"	"natural"	"tone"
"contain"	"needle"	"typic"
"crucible"	"neutral"	"usp"
"cryst"	"nitrile"	"wire"
"deriv"	"pearl"	"with"
"dispers"	"pellet"	"xime"
"dry "	"piece"	"zone"
"dust"	"plate"	
"ed "	"poly"	
"electro"	"porous"	
"ester"	"powder"	
"ether"	"ppm"	
"fcc"	"pract"	
"fine"	"predomina"	
"flake"	"predominantly"	
"foil"	"protected"	
"for "	"puratronic"	
"from"	"pure"	
"glacial"	"purity"	
	"purum"	

FIG. 5C

Table 4.

ether
sulfide
disulfide
trisulfide
tetrasulfide
pentasulfide
hexasulfide
selenide
diselenide
triselenide
telluride
sulfone
disulfone
trisulfone
sulfoxide
disulfoxide
trisulfoxide
peroxide
ketone
diketone
triketone
tetraketone

FIG. 5D

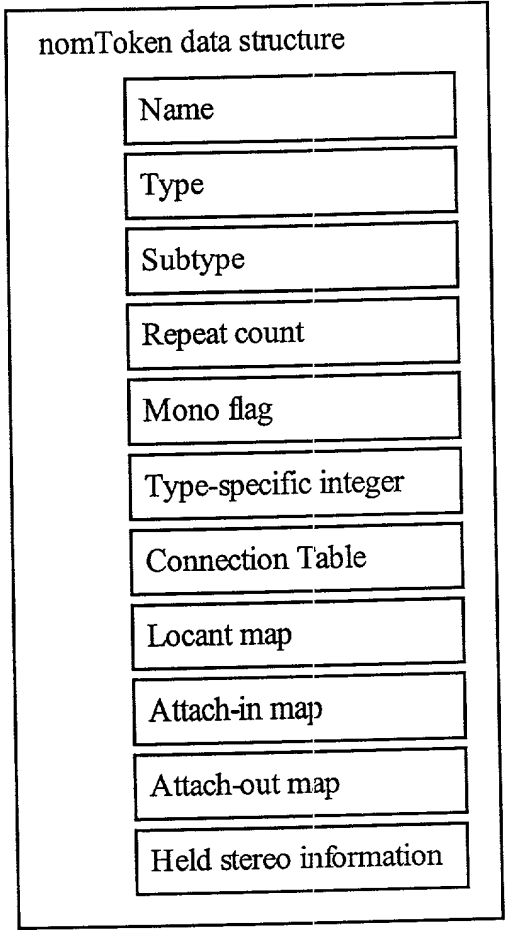


FIG. 6

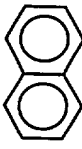

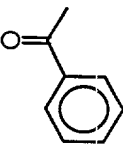


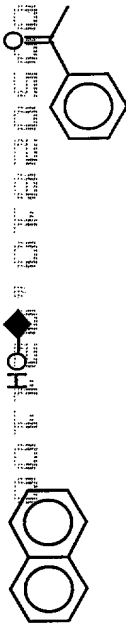
CONNECTION TABLE			
NAME			
TYPE	p		
SUBTYPE	unknown		
PREV CHAR	'('		
			
	naphth	oxy	phenac
	opfuser	infix	root
	unknown	doublebondable	root
	'a'	'a'	'a'
			
			yl
			enderaminoacid
			yl
			'a'
			
			bromide
			counterion
			ionable
			'a'

FIG. 7A

CONNECTION TABLE

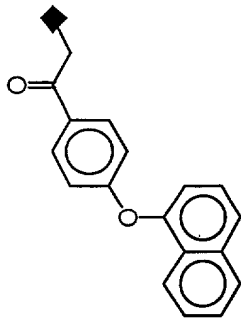
NAME	p	naphth	oxy	phenac	bromide
TYPE	unknown	root	infix	root	counterion



SUBTYPE	unknown	unknown	doublebondable	yl	ionable
PREV CHAR	'('	'a'	'a'	'a'	' '

FIG. 7C

CONNECTION
TABLE



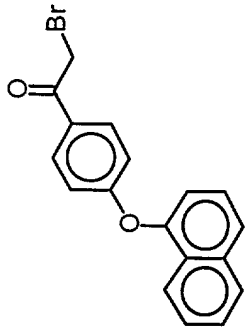
NAME p-naphthoxy-phenacyl
TYPE root
SUBTYPE root
PREV CHAR 'a'



bromide
counterion
ionable
, ,

FIG. 7F

CONNECTION
TABLE



NAME p-naphthoxy-phenacyl bromide
 TYPE root
 SUBTYPE root
 PREV CHAR 'a'

FIG. 76

DECLARATION AND POWER OF ATTORNEY
(Attorney Docket No. 103544.127)

As a below-named inventor, I hereby declare that:

My residence, post office address and citizenship is as stated below next to my name.

I believe that I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled:

DERIVING CHEMICAL STRUCTURAL INFORMATION

the specification of which (check only one):

- ☒ is attached hereto.
- ☐ was filed as United States Patent Application
Serial No. _____
and was amended
on _____
(if applicable)
- ☐ was filed as PCT Patent Application
Serial No. _____
on _____
and was amended under PCT Article 19
on _____
(if applicable)

I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to the patentability of the claims of this application in accordance with Title 37, Code of Federal Regulations, Sections 1.56(a) and 1.56(b).

I hereby claim foreign priority benefits under Title 35, United States Code, § 119(a)-(d) or 365(b) of any foreign application(s) for patent or inventor's certificate or of any PCT international application(s) designating at least one country other than the United States of America listed below and have also identified below any foreign application(s) for patent or inventor's certificate or any PCT international application(s) designating at least one country other than the United States of America filed by me on the same subject matter having a filing date before that of the application(s) of which priority is claimed:

EXPRESS MAIL LABEL NO. EM259723548US
DATE OF DEPOSIT February 11, 2000

**PRIOR FOREIGN/PCT APPLICATION(S) AND ANY PRIORITY CLAIMS
UNDER 35 U.S.C. §119(a)-(d) or 365(b):**

COUNTRY (if PCT indicate PCT)	APPLICATION NUMBER	DATE OF FILING	PRIORITY CLAIMED UNDER 35 U.S.C. §119(a)-(b) or 365(b) (YES/NO)
--	---------------------------	-----------------------	---

I hereby claim the benefit under 35 U.S.C. §119(e) of any United States provisional patent application(s) listed below:

APPLICATION NUMBER	DATE OF FILING	STATUS: (PENDING OR ABANDONED)
60/119,930	February 12, 1999	PENDING

I hereby claim the benefit under Title 35, United States Code, § 120 or 365(c) of any United States application(s) or PCT international application(s) designating the United States of America that is/are listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in that/those prior application(s) in the manner provided by the first paragraph of Title 35, United States Code, § 112. I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, § 1.56 which occurred between the filing date of the prior applications and the national or PCT international filing date of this application:

**PRIOR U.S. APPLICATION OR PCT INTERNATIONAL APPLICATION(S)
DESIGNATING THE U.S. FOR BENEFIT UNDER 35 U.S.C. § 120 or 365(c):**

APPLICATION NUMBER	DATE OF FILING (day, month, year)	STATUS: (PATENTED, PENDING OR ABANDONED)
---------------------------	---	---

POWER OF ATTORNEY: As named inventors, we hereby appoint the following attorneys and/or agents to prosecute this application and transact all business in the Patent and Trademark Office connected therewith

Michael J. Bevilacqua	Reg. No. 31,091
James B. Lampert	Reg. No. 24,564
Wayne M. Kennard	Reg. No. 30,271
Hollie L. Baker	Reg. No. 31,321
Wayne A. Keown	Reg. No. 33,923
Donald R. Steinberg	Reg. No. 37,241
Michael A. Diener	Reg. No. 37,122
Richard A. Goldenberg	Reg. No. 38,895

Peter M. Diciara	Reg. No. 38,005
Ann-Louise Kerner	Reg. No. 33,523
Colleen Superko	Reg. No. 39,850
Gretchen Rice	Reg. No. 37,429
Keum J. Park	Reg. No. 42,059
Jason A. Reyes	Reg. No. 41,513
Janice M. Klunder	Reg. No. 41,121
Henry N. Wixon	Reg. No. 32,073
Barbara A. Barakat	Reg. No. 32,190
Nancy Chiu	Reg. No. 43,545
Rajesh Vallabh	Reg. No. 35,761
Ayla A. Lari	Reg. No. 43,739

the mailing address and telephone number of each of whom is HALE AND DORR LLP, 60 State Street, Boston, Massachusetts 02109 and (617) 526-6000, with full power of substitution and revocation to prosecute this application and to transact all business in the Patent and Trademark Office connected therewith.

Send Correspondence To

**Jason A. Reyes
Hale and Dorr LLP
60 State Street
Boston, MA 02109**

Direct Telephone Calls To

**Jason A. Reyes
(617) 526-6010**

Wherefore I petition that letters patent be granted to me for the invention or discovery described and claimed in the attached specification and claims, and hereby subscribe my name to said specification and claims and to the foregoing declaration, power of attorney, and this petition.

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

Full name of sole inventor: Jonathan S. Brecher

Inventor's signature _____ Date _____

Country of Citizenship: USA

Residence: 52 Montgomery Street, #2, Cambridge, MA 02140

Post Office Address: _____

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant: Jonathan Scott Brecher

Serial No.: To Be Assigned

Filed: Herewith (This application claims the benefit of U.S. Provisional Application Serial No. 60/119,930 entitled DERIVING A CHEMICAL STRUCTURE FROM A CHEMICAL NAME, filed on February 12, 1999.)

Title: DERIVING CHEMICAL STRUCTURAL INFORMATION

Box Patent Application
Assistant Commissioner for Patents
Washington, DC 20231

COVER SHEET FOR APPENDIX: NOMTOKENS

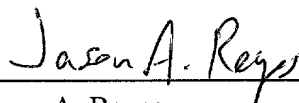
Dear Sir:

Enclosed for filing in the above-referenced patent application is the following document:

1. Appendix: NOMTOKENS, 111 pages.

The following is the inventor's residence:
52 Montgomery Street, #2, Cambridge, MA 02140.

Respectfully submitted,



Jason A. Reyes
Registration No. 41,513
Attorney for Applicant

Dated: February 11, 2000

Hale and Dorr LLP
60 State Street
Boston, MA 02109
Tel.: (617) 526-6010
Fax: (617) 526-5000

Attorney Docket No. 103544.127

EXPRESS MAIL LABEL NO. EM259723548US
DATE OF DEPOSIT February 11, 2000

00502910 021100

meth|carbin root alkane C,a|alpha|1|w|omega
 carbenium root root [C+],1|w|omega
 carbene root root C,32@1|w|omega
 aminylene|nitrene root root N,32@1|w|omega
 hydroxymethyl root root C,4@x,O,x
 hydroxymethylene root root C,8@x,O,x
 form root trivial C,x|1|w|omega,(=O),x
 formimino root trivial C,4@x|1|w|omega,(=N),x
 formalin root root C=O,x
 eth root alkane C,1|a|alpha,C,2|b|beta|w|omega
 ethene|ethen root alkane C,1|a|alpha,=,x,C,2|b|beta|w|omega
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 hexafluoroisoprop|hexafluoroisopropa root alkane
 C,a|alpha,(C(F)(F)F),x,C(F)(F)F,x
 propiono|propion|propio|propi root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta|w|omega
 proparg|proparag root alkane C,1|a|alpha,C,2,#,x,C,3|w|omega
 tetrol|loveracid alkane C,1,C,2,#,x,C,3,C,4|w|omega
 but|buta root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma,C,4|d|delta|w|omega
 butyro|butyr root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma|w|omega
 isobutyro|isobutyr root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4|b'|beta'|g|gamma|w|omega
 isobutylene root root C=C(C)C,x
 crotono|croton root trivial
 C,1,(=,x,O,x),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 crot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 crotonylalcohol root root
 C,1,(O),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 isocrotono|isocroton root trivial
 C,1,(=,x,O,x),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 isocrot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 seneci root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,=,x,C,3|b|beta,(,x,C,4|g|gamma|w|omega,),x,C,4'|g'|gamma'|w'|omega'
 tigl|cevad root trivial
 C,1,(=,x,O,x),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 angel root trivial
 C,1,(=,x,O,x),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 pren root alkane C,1,C,2|a|alpha,=,x,C,3|b|beta,(C),x,C,4|g|gamma|w|omega
 valero|valer|valerian root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
 acetonoal root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,(=O),x,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta|w|omega
 valpr root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,(CCC),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
 levulin|laevulin|levul root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4,(=O),x,C,5|g|gamma|d|delta|w|omega
 isovalero|isovaler|delphin root trivial
 C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,(,x,C,4|g|gamma,),x,C,5|d|delta|w|omega

pival root trivial
 $C,1,(=,x,0,x),x,C,2|a|alpha,(x,C,3|b|beta),(x,C,4|3',),x,C,5|3''$
 amyl root alkane $C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega$
 capro root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon|w|omega$
 acexam root root
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=0),x,C,x,$
 enatho|enanth|oenantho|oenanth root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7|w|omega$
 geron root trivial
 $C,1,(=,x,0,x),x,C,2|a|alpha,(C)(C),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=0),x,C,7|w|omega$
 capryl root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8|w|omega$
 octoate root root
 $O,1@x,C,1,(=0),x,C,2|a|alpha,(x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,n),x,C,x,C,x$
 pelargono|pelargon|pelarg|pergon root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9|w|omega$
 capr root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 obtusil root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 stilling root alkane
 $C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma,=,x,C,5|d|delta,\backslash,x,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 lauro|laur|vulv|laurostear root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12|w|omega$
 linder root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12|w|omega$
 myristo|myrist root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 physeter|physoter root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,=,x,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 ipurol root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,(0),x,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,(0),x,C,12,C,13,C,14|w|omega$
 tsuzu|tudu root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 myristelaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,=,x,C,10,/,x,C,11,C,12,C,13,C,14|w|omega$
 myristole root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,=,x,C,10,\backslash,x,C,11,C,12,C,13,C,14|w|omega$
 palmito|palmit|cet root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega$

jalapinol root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,(O),x,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 ole root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 elaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 ricinole|ricinol root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 ricinelaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 linole|telfair root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega$
 vernol loveracid root CCCCCC\C=C/C[C@H]1[C@H](CCCC)O1,x
 linolelaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega$
 linolenelaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,/,x,C,17,C,18|w|omega$
 linolen|alphalinolen root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,/,x,C,17,C,18|w|omega$
 gammalinolen root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega$
 vaccen root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,/,x,C,11,/,x,C,12,/,x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 petroselaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 petroselin root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega$
 calend root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega$
 arachido|arachid|arachin root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega$
 gadole root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega$
 arachidon root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,/,x,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,C,17,C,18,C,19,C,20|w|omega$


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methacr root trivial C,1,(=,x,O,x),x,C,2,(x,C,4),x,=,x,C,3|w|omega
propiol root trivial C,1,(=,x,O,x),x,C,2,#,x,C,3
glyoxal root trivial C,1,(=,x,O,x),x,C,2,=,x,O,x
oxalo|oxal root diacid C,1,(=,x,O,x),x,C,4@2,=,x,O,x
oxamid|oxam root trivial C,1,(=,x,O,x),x,C,2,(x,N,n),x,=,x,O,x
oxanil root trivial
C,1,(=,x,O,x),x,C,2,(x,N,n,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
),x,=,x,O,x
mucochlor root trivial
C,1,(=,x,O,x),x,C,2|a|alpha,(Cl),x,=,x,C,3|b|beta|w|omega,(Cl),x,C=O,x
mucobrom root trivial
C,1,(=,x,O,x),x,C,2|a|alpha,(Br),x,=,x,C,3|b|beta|w|omega,(Br),x,C=O,x
pyromuc root root C,x,c,x,Ring,Ring1,c,x,c,x,c,x,o,x,Ring,Ring1
malono|malon root diacid C,1,(=,x,O,x),x,C,2|w|omega,C,4@3,=,x,O,x
tartrono|tartron root diacid C,1,(=,x,O,x),x,C,2,(x,O,x),x,C,4@3,=,x,O,x
mesoxal root diacid C,1,(=,x,O,x),x,C,2,(=,x,O,x),x,C,4@3,=,x,O,x
mesoxalo root root C,4@1,(=,x,O,x),x,C,2,(=,x,O,x),x,C,3,(x,O,x),x,=,x,O,x
oxalacet root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3,(=,x,O,x),x,C,4@4|w|omega,=,x,O,x
oxalaceto root diacid
C,4@1,(=,x,O,x),x,C,2|a|alpha,C,3,(=,x,O,x),x,C,4,(x,O,x),x,=,x,O,x
succino|succin root diacid C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4@4,=,x,O,x
isosuccino|isosuccin root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,(x,C,3|b|beta),x,C,4@4,=,x,O,x
caron root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,(C(C)(C),x,Ring,Ring1),x,C,3|b|beta,Ring,Ring1,C,4
@4,=,x,O,x
male|malen|malein|toxil root diacid
C,1,(=,x,O,x),x/,x,C,2,=,x,C,3,\,x,C,4@4,=,x,O,x
fumar|bolet root diacid C,1,(=,x,O,x),x/,x,C,2,=,x,C,3/,x,C,4@4,=,x,O,x
maleur root trivial C,1,(=,x,O,x),x/,x,C,2,=,x,C,3,\,x,C,4,N,x,C,x,(=O),x,N,x
citracon root diacid C,1,(=,x,O,x),x/,x,C,2,(C),x,=,x,C,3,\,x,C,4@4,=,x,O,x
mesacon root diacid C,1,(=,x,O,x),x/,x,C,2,(C),x,=,x,C,3/,x,C,4@4,=,x,O,x
teracon root diacid C,1,(=,x,O,x),x,C,2,(=C(C)C),x,C,3,C,4@4,=,x,O,x
mal root diacid C,1,(=,x,O,x),x,C,2,(x,O,x),x,C,3,C,4@4,=,x,O,x
citramal root diacid C,1,(=,x,O,x),x,C,2,(x,O,x)(x,C,x),x,C,3,C,4@4,=,x,O,x
pyrotartr|pyrotartar root diacid
C,1,(=,x,O,x),x,C,2,(x,C,x),x,C,3,C,4@4,=,x,O,x
itacon root diacid C,1,(=,x,O,x),x,C,2,(=,x,C,x),x,C,3,C,4@4,=,x,O,x
tartar|tartr|dtartar|dtartr|uv|mesotartar|mesotartr pseudosugar unknown x,x
tartar|tartr|uv root diacid
C,1,(=O),x,Ring,Ring1,.x,O,o,Ring,Ring2,.x,O,o',Ring,Ring3,.x,C,2,Ring,Ring1,
Ring,Ring2,C,3,Ring,Ring3,C,4@4,=,x,O,x
dtartar|dtartr root diacid
C,1,(=O),x,Ring,Ring1,.x,O,o,Ring,Ring2,.x,O,o',Ring,Ring3,.x,[C@H],2,Ring,Ri
ng1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
ltartar|ltartr root diacid
C,1,(=O),x,Ring,Ring1,.x,O,o,Ring,Ring2,.x,O,o',Ring,Ring3,.x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@@H],3,Ring,Ring3,C,4@4,=,x,O,x
mesotartar|mesotartr root diacid
C,1,(=O),x,Ring,Ring1,.x,O,o,Ring,Ring2,.x,O,o',Ring,Ring3,.x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
him root diacid
C,x,(=,x,O,x),x,C,2,Ring,Ring1,C,3,(x,C,4,Ring,Ring2,C,5,=,x,C,6,C,1,(x,C,7,R
ing,Ring2),x,Ring,Ring1),x,C,4@x,=,x,O,x
glutaro|glutar root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,4@5,=,x,O,x

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adipo|adip root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,4@6,=,x,0,x$
 glutacon|glutacono root diacid $C,1,(=,x,0,x),x,C,2,=,x,C,3,C,4,C,4@5,=,x,0,x$
 mucon|mucono root diacid $C,1,(=,x,0,x),x,C,2,=,x,C,3,C,4,=,x,C,5,C,4@6,=,x,0,x$
 dihydromucon|dihydromucono root diacid
 $C,1,(=,x,0,x),x,C,2,=,x,C,3,C,4,C,5,C,4@6,=,x,0,x$
 pimelo|pimel|piler root diacid
 $C,1,(=,x,0,x),x,C,2,C,3,C,4,C,5,C,6,C,4@7,=,x,0,x$
 subero|suber root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,4@8,=,x,0,x$
 azela|azele|azel|lepargyl root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,4@9,=,x,0,x$
 sebaco|sebac root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,4@10,=,x,0,x$
 traumat|traumato root diacid
 $C,1,(=,x,0,x),x,C,2,=,x,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,4@12,=,x,0,x$
 brassylo|brassylo root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,4@13,=,x,0,x$
 thapso|thaps root diacid
 $C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,4@16,=,x,0,x$
 floion|phloion root diacid
 $C,1,(=,x,0,x),x,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,(O),x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,4@18,=,x,0,x$
 folin root diacid
 $C,x,(=,x,0,x),x,(C(CC,x,C,4@x,=O)NC(C(C=C3)=CC=C3NCC(CN2)N(C=O)C1=C2N=C(N)NC1=O)=O),x$
 spiculspor root diacid
 $C,x,(=,x,0,x),x,ring,ring1,.,x,C,1,(x,=,x,0,x),x,(x,0,x,ring,ring2),x,C,2,C,3,C,4,ring,ring2,ring,ring1,C,5,(x,C,4@x,=,x,0,x),x,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15$
 chaulmoogr root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,[C@@H],x,ring,ring1,c,x,c,x,C,x,C,x,ring,ring1$
 pyrocarbon root diacid $C,x,(=,x,0,x),x,0,x,C,4@x,=,x,0,x$
 imidodicarbon|iminodicarbon root diacid $C,x,(=,x,0,x),x,N,n,C,4@x,=,x,0,x$
 pyrocarbon root diacid $C,x,(=,x,0,x),x,0,x,C,4@x,=,x,0,x$
 thiodicarbon root diacid $C,x,(=,x,0,x),x,S,x,C,4@x,=,x,0,x$
 peroxydicarbon root diacid $C,x,(=,x,0,x),x,OO,x,C,4@x,=,x,0,x$
 thioperoxydicarbon root diacid $C,x,(=,x,0,x),x,SS,x,C,4@x,=,x,0,x$
 chelidon|chelid root diacid $C,x,(=,x,0,x),x,c1cc(=O)cc(o1),x,C,4@x,=,x,0,x$
 pamo|embon root diacid
 $C,x,(=,x,0,x),x,C1=CC3=C(C=CC=C3)C(CC2=C(C=CC=C4)C4=CC(,x,C,4@x,=,x,0,x)=C2O)=C1O,x$
 citr root polyacid $C,1,C,2,C,3,(x,0,x),x,(x,C,x),x,C,x,C,x$
 isocitr root polyacid $C,x,C,x,(x,0,x),x,C,x,(x,C,x),x,C,x,C,x$
 tricarballyl root polyacid $C,x,C,x,C,x,(x,C,x),x,C,x,C,x$
 aconit root polyacid $C,x,C,x,=,x,C,x,(x,C,x),x,C,x,C,x$
 trimellit root polyacid
 $C,x,c,1,ring,ring1,c,2,(x,C,x),x,c,3,c,4,c,5,(x,C,x),x,c,6,ring,ring1$
 hemimellit root polyacid
 $C,x,c,1,ring,ring1,c,2,(x,C,x),x,c,3,(x,C,x),x,c,4,c,5,c,6,ring,ring1$

hemimellitene root root
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, (, x, C, x,), x, c, 4, c, 5, c, 6, Ring, Ring1
pyromellit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, c, 4, (, x, C, x,), x, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
pyromellitene root root
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, c, 4, (, x, C, x,), x, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
mellit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, (C), x, c, 6, (C), x, Ring, Ring1
trimes root polyacid
C,x,c,1, Ring, Ring1, c, 2, c, 3, (, x, C, x,), x, c, 4, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
mellophan root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, c, 6, Ring, Ring1
prehnit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, c, 5, (C), x, c, 6, Ring, Ring1
berberon|beron root polyacid
C,x,c,2, Ring, Ring1, c, 3, (, x, C, x,), x, c, 4, c, 5, (, x, C, x,), x, c, 6, n, 1, Ring, Ring1
phthalide root root
O,x,=,x,C,1, Ring, Ring1, O, 2, C, 3|a|alpha, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
phthalane|phthalan root root
C, 1, Ring, Ring1, O, 2, C, 3, C, 3a, Ring, Ring2, =, x, C, 4, C, 5, =, x, C, 6, C, 7, =, x, C, 7a, Ring, Ring1, Ring, Ring2
phthalo|phthal|orthophthal root diacid
C,x,(=,x,O,x,), x, c, 1, Ring, Ring1, c, 2, (, x, C, 4@x, =, x, O, x,), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
homophthalo|homophthal root diacid
C,x,(=,x,O,x,), x, c, 1, Ring, Ring1, c, 2, (, x, C, x, C, 4@x, =, x, O, x,), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
isophthalo|mpthalo|isophthal|mpththal root diacid
C,x,(=,x,O,x,), x, c, 1, Ring, Ring1, c, 2, c, 3, (, x, C, 4@x, =, x, O, x,), x, c, 4, c, 5, c, 6, Ring, Ring1
terephthalo|ppthalo|terephthal|ppththal root diacid
C,x,(=,x,O,x,), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, (, x, C, 4@x, =, x, O, x,), x, c, 5, c, 6, Ring, Ring1
uvit root diacid
C,x,(=,x,O,x,), x, c, 1, Ring, Ring1, c, 2, c, 3, (, x, C, 4@x, =, x, O, x,), x, c, 4, c, 5, (C), x, c, 6, Ring, Ring1
leucate|leucicacid root root
C, 1, (=,x,O,x,), x, (, x, O, 1@x,), x, C, 2, (, x, O, x,), x, C, 3, C, 4, (, x, C, 5,), x, C, x
phenylephrine|phenylephrin root root Oc1cccc(C(O)CNC)c1,x
norepinephrine|norepinephrin|noradrenaline|noradrenalin|arterenol root root Oc1cc(C(O)CN)ccc1O,x
epinephrine|epinephrin|adrenaline|adrenalin root root Oc1cc(C(O)CNC)ccc1O,x
adrenalone root root O=C(CNC)c1ccc(O)c(O)c1,x
norephedrine|norephedrin root root OC(C(,x,N,n,C)C),x,c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
ephedrine|ephedrin|pseudoephedrine|pseudoephedrin root root OC(C(,x,N,n,C)C),x,c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
taurine|taurin root root C,1@x,S,x,(=O)(=O),x,C,1,C,2,N,n
hypotaurine|hypotaurin root root O,1@x,S,x,(=O),x,C,1,C,2,N,n
cadaverine|cadaverin root root N,n,C,1,C,2,C,3,C,4,C,5,N,n'
putrescine|putrescin root root N,n,C,1,C,2,C,3,C,4,N,n'

albizzi aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, NC(=O)N, x

alan aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta
 homoalan aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | d | delta | w
 | omega
 alanos aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, N, x, (, x, O, x,)
 , x, N, x, =, x, O, x
 alloisoleuc aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, [C@H], 2 | a | alpha, Ring, Ring1, [C@@H], 3 | b | beta, (, x,
 C, 4 | g | gamma, C, 5 | d | delta,) , x, C, 3',
 allothreon aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, [C@H], 2 | a | alpha, Ring, Ring1, [C@H], 3 | b | beta, (, x, C
 , 4 | g | gamma,) , x, O, x
 allys aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
 , 5 | d | delta, C, 6 | e | epsilon, =O, x
 argin aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
 , 5 | d | delta, N, nd | ndelta, C, x, (=, x, N, nw' | nomega',) , x, N, nw | nomega | ngamma
 asparag aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, (
 =, x, O, x,) , x, N, ngamma
 aspart aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3, C, 4 | g | gamma | b | beta, (
 =, x, O, x,) , x, O, x
 azaser aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, O, x, C (=O) C = [N
 +] = [N-], x
 betaalan aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nbeta | n3, C, 2 | a | alpha, C, 3 | b | beta, Ring, Ring1
 buthion aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S
 , x, CCCC, x
 canavan aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, O
 NC (=N) N, x
 carbocyste aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s, CC (=O), x,
 O, 1@x
 citrull aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
 , 5 | d | delta, N, x, C, x, (=, x, O, x,) , x, N, x
 cycloleuc aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, Ring, Ring2, C, 3 | b | beta, C,
 4 | g | gamma, C, 5 | d | delta, C, 6, Ring, Ring2
 cyste reqineaminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s
 cyste aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s, (=O) (=O),
 x, O, 1@x,
 ethion aminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S
 , x, C, x, C, x
 isoglutam reqineaminoacid ine
 C,1, Ring, Ring1, ., x, N, n | nalpha | n2, Ring, Ring2, ., x, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | bet
 a, C, 4 | g | gamma, Ring, Ring2, C, 5 | d | delta, (=, x, O, x,) , x, N, x

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glutam reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, C
, 5|d|delta, (=, x, O, x, ), x, N, nd|ndelta|n5
glutam aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, C
, 5|d|delta, (=, x, O, x, ), x, O, 1@x
glyc aminoacid ine C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1
histid aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, c, 4, Ring, Ring2, c,
5, n, 1|nt|ntau|im|nim|n'|tau|prefhydro, c, 2, n, 3|np|npi, Ring, Ring2
homoargin aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, C
, 5|d|delta, C, 6|e|epsilon, N, nd|ndelta, C, x, (=, x, N, nw'|nomega', ), x, N, nw|nomega
homocitrull aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, C
, 5|d|delta, C, 6|e|epsilon, N, x, C, x, (=, x, O, x, ), x, N, x
homocyste reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, S
, s
homocyste aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, S
, s, (=O) (=O), x, O, 1@x
homoglutam reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, C
, 5|d|delta, C, 6|e|epsilon, (=, x, O, x, ), x, N, ne|nepsilon|n6
homophenylalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, g|gamma, c, x, Rin
g, Ring2, c, 2|o|ortho, c, 3|m|meta, c, 4|p|para, c, 5, c, 6, Ring, Ring2
homoprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1|n|nalpha|n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, C, 6, Rin
g, Ring2
homoser aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, O
, x
homotryptoph aminoacid ane
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, g|gamma, C, 3, Rin
g, Ring2, =, x, C, 2, N, 1, C, 7a, Ring, Ring3, =, x, C, 7, C, 6, =, x, C, 5, C, 4, =, x, C, 3a, Ring, Ring2,
Ring, Ring3
iboten aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C2=CC(=O)NO2, x
isoleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, [C@H], 2|a|alpha, Ring, Ring1, [C@H], 3|b|beta, (, x, C
, 4|g|gamma, C, 5|d|delta, ), x, C, 3',
isoser aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, Ring, Ring2, ., x, C, 2|a|alpha, Ring, Ring1, (O), x, C, 3
|b|beta, Ring, Ring2
isoval aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, (, x, C, 2', ), x, Ring, Ring1, C, 3|b|beta,
C, 4|g|gamma
kynuren aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C(=O), x, c, 1, Ring,
Ring2, c, 2, (N), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring2
leuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, C, 4|g|gamma, (
, x, C, 5|d|delta, ), x, C, 5'

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lys aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, C, 6 | e | epsilon, N, n6 | nw | nomega | nep | n | ne | nz | n'
methion aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S, x, C, x
mimos aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, N2C=C(O)C(=O)C=C2, x
norleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, C, 6 | e | epsilon
norval aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta
ornith aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, N, n5 | ndelta | nd
penicillam aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, (C) (C) S, x
phenylalan|3phenylalan|betaphenylalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, c, x, Ring, Ring2, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring2
prol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, Ring, Ring2
3hydroxyprol|hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | ralpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, (O), x, C, 4, C, 5, Ring, Ring2
4hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | ralpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, (O), x, C, 5, Ring, Ring2
5hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | ralpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, (O), x, Ring, Ring2
pyroglutam aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, (=O), x, Ring, Ring2
sarcos aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, (, x, C, 2 | a | alpha, Ring, Ring1, ) , x, C, x
selenocyste regineaminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, [Se], se
selenomethion aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, [Se], x, C, x
ser aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, O, x
tleuc|tertleuc aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, (, x, C, 3', ) (, x, C, 3'', ) , x, C, 3'''
theano|thean aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, x, (=O), x, N, x, C, x, C, x
thiocitrull aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, N, x, C, x, (=, x, S, x, ) , x, N, x

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threono|threon aminoacid ine
C,1, Ring, Ring1, ., x, N, n|nalpha|n2, [C@H], 2|a|alpha, Ring, Ring1, [C@H], 3|b|beta, (, x,
C, 4|g|gamma, ), x, O, x
tryptoph aminoacid ane
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 3, Ring, Ring2, =,
x, C, 2, N, 1, C, 7a, Ring, Ring3, =, x, C, 7, C, 6, =, x, C, 5, C, 4, =, x, C, 3a, Ring, Ring2, Ring, Ring3
thyron aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 1, Ring, Ring2, =,
x, C, 2|ortho, C, 3|m|meta, =, x, C, 4, (, x, O, x, C, 1', Ring, Ring3, =, x, C, 2', C, 3', =, x, C, 4', (,
x, O, x, ), x, C, 5', =, x, C, 6', Ring, Ring3, ), x, C, 5, =, x, C, 6, Ring, Ring2
thyrox aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 1, Ring, Ring2, =,
x, C, 2|ortho, C, 3|m|meta, (I), x, =, x, C, 4, (, x, O, x, C, 1', Ring, Ring3, =, x, C, 2', C, 3', (I), x,
=, x, C, 4', (, x, O, x, ), x, C, 5', (I), x, =, x, C, 6', Ring, Ring3, ), x, C, 5, (I), x, =, x, C, 6, Ring,
Ring2
tyros|ptyros|paratyros aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 1, Ring, Ring2, =,
x, C, 2|ortho, C, 3|m|meta, =, x, C, 4, (, x, O, x, ), x, C, 5, =, x, C, 6, Ring, Ring2
mtiros|metatyros aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 1, Ring, Ring2, =,
x, C, 2|ortho, C, 3|m|meta, (, x, O, x, ), x, =, x, C, 4, C, 5, =, x, C, 6, Ring, Ring2
orthotyros aminoacid ine
C, x, Ring, Ring1, ., x, N, n|nalpha|n2, C, a|alpha, Ring, Ring1, C, b|beta, C, 1, Ring, Ring2, =,
x, C, 2|ortho, (, x, O, x, ), x, C, 3|m|meta, =, x, C, 4, C, 5, =, x, C, 6, Ring, Ring2
val aminoacid ine
C, 1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, (, x, C, 4|g|gam
ma, ), x, C, 4'|5
willardi aminoacid ine
C, 1, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta, n2ccc(=O)nc(=
O)2, x
djenkol aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
S, x, C, x, S, x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =, x, O, x
cyst aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
S, x, S, x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =, x, O, x
cystathion aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
C, 4|g|gamma, S, x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =, x,
O, x
homocyst aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
C, 4|g|gamma, S, x, S, x, C, 4'|g'|gamma', C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nal
pha', ), x, C, 4@x, =, x, O, x
lanthion aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
S, x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =, x, O, x
selenocyst aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
[Se], x, [Se], x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =, x, O,
x
selenocystathion aminodiacid ine
C, 1, (=, x, O, x, ), x, Ring, Ring1, ., x, N, n|nalpha|n2, C, 2|a|alpha, Ring, Ring1, C, 3|b|beta,
C, 4|g|gamma, [Se], x, C, 3'|b'|beta', C, 2'|a'|alpha', (, x, N, n'|na'|nalpha', ), x, C, 4@x, =
, x, O, x
in|ine enderaminoacid ine 0,8@x, ., x, O, 5@x
an|ane enderaminoacid ane 0,8@x, ., x, O, 5@x

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[illegible]

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allo sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,6
,O,x
altro|altr sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x),x,[C@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
gluco|gluc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
manno|mann sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
gulo|gul sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
ido sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x),x,[C@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
galacto|galact|dulc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
talo|tal sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,
C,6,O,x
boivin sugar hexose
O,x,=,x,C,1,[C@H](,2,[C@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,6
digitox sugar hexose
O,x,=,x,C,1,C,2,[C@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,6
oli sugar hexose
O,x,=,x,C,1,[C@H](,2,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,6
oliv sugar hexose
O,x,=,x,C,1,[C@H](,2,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,6
glucohept sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@H](,3,O,x),x,[C@H](,4,O,x),x,[C@@H](,5,O,x)[C
@H](,6,O,x),x,C,7,O,x
fuco|fuc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6
quinovo|quinov sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6
rhamno|rhamn sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6
rhodeo|rhode sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x),x,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6
thymino|thymin sugar hexose
O,x,=,x,C,1,[C@H](,2,[C@H](,3,O,x),x,[C@H](,4,O,x),x,C,5,O,x
galactosamine|galactosamin|chondrosamine|chondrosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x),x,[C@@H](,3,O,x),x,[C@@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x
glucosamine|glucosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x),x,[C@@H](,3,O,x),x,[C@H](,4,O,x)[C@H](,5,O,x),x,C,
6,O,x

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mannosamine|mannosamin sugar trivial
O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
fucosamine|fucosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
quinovosamine|quinovosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6
rhamnosamine|rhamnosamin sugar trivial
O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
glucal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
rhamnal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6
galactal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
glucamine sugar trivial
N,n,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6,O,
x

sucr sugar disugar
OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)
)O2,x
trehal sugar disugar
O[C@H]1[C@H](O)[C@@H](CO)O[C@H](O[C@H]2[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O2)[C@
H]1O,x
melezit sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O[C@@H]2(CO)[C@@H](O[C@H]3O[C@H](CO)[C@
H](O)[C@H](O)[C@H]3O)[C@H](O)[C@@H](CO)O2)O1,x
stachy|lupe sugar disugar
O[C@H]1[C@@H](CO)O[C@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O[C@H]4(CO)O[C@H](CO)[C@@H](
O)[C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@H]2O)[C@H](O)[C@H]1O,
x
lact sugar disugar
OC[C@H]1O[C@@H](O[C@@H]([C@H](O)[C@@H](O)[C@@H](O)O2)[C@H]2CO)[C@H](O)[C@@H](O)[
C@H]1O,x
malt|maltobi sugar disugar
O[C@@H]1[C@@H](O)[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)O[C@H](CO)[C
@H]1O,x
maltotri sugar disugar
O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]1O[C@@H]2[C@@H](CO)O[C@H](O[C@@H]3[C@@
H](CO)OC(O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O,x
maltotetra sugar disugar
O[C@@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O)O[C@@H]4CO)O)O[C@@H]1CO)[C@@H](O)[C
@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]3O)[C@H](O)[C@H]3O)[C@@H
](CO)O2)O,x
maltopenta sugar disugar
O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1[C@@H](CO)O[C@H](O[C@H]3[C@H](O)[
C@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O[C@H]5[C@H](O)[C@H]([C@@H](O)O[C@@H]5CO
)O)O[C@@H]4CO)O)O[C@@H]3CO)O)[C@H](O)[C@H]1O,x
maltohexa sugar disugar
O[C@@H]([C@@H](O[C@H]3[C@H](O)[C@H]([C@@H](O[C@H]6[C@H](O)[C@H]([C@@H](O)O[C@@H]
6CO)O)O[C@@H]3CO)O)O[C@@H]1CO)[C@@H](O)[C@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H
]4[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]5O)[C@H](O)[C@H]5O)[C@@H](CO)O4)O)[
C@@H](CO)O2)O,x

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melibi sugar disugar
O[C@H]1[C@@H](OC[C@H]([C@@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@H](O)[C@@H]
10,x
cellobi sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O)[C@H](O)[C@
H]2O)O1,x
cellotri sugar disugar
O[C@H]([C@H]1O)[C@H](O[C@H]2[C@H](O)[C@H]([C@H](O[C@H]3[C@H](O)[C@H](C(O)O[C@@H]
3CO)O)O[C@@H]2CO)O)O[C@H](CO)[C@H]1O,x
cellotetra sugar disugar
OC(O[C@@H](CO)[C@@H]1O[C@H]2[C@@H](O)[C@H](O)[C@@H](O[C@@H]3[C@@H](O)[C@H](O)[C@
H](O[C@@H]4[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O4)[C@H](CO)O3)[C@H](CO)O2)[C@@H]
(O)[C@@H]1O,x
cellopenta sugar disugar
OC(O[C@H]1CO)[C@@H](O)[C@@H]([C@H]1O[C@H]2[C@@H](O)[C@H](O)[C@@H](O[C@H](O[C@@H]
(CO)[C@@H]3O[C@@H]4[C@@H](O)[C@H](O)[C@@H](O[C@@H]5[C@@H](O)[C@H](O)[C@@H](O)[C@
H](CO)O5)[C@H](CO)O4)[C@@H](O)[C@@H]3O)[C@H](CO)O2)O,x
chitobi sugar disugar
N,n,[C@@H]([C@H](O)O[C@@H]2CO)[C@@H](O)[C@@H]2O[C@H](O1)[C@H](,x,N,n',)[C@@H](O)
[C@H](O)[C@H]1CO,x
chitotri sugar disugar
N,n,[C@@H](C(O)O[C@@H]3CO)[C@@H](O)[C@@H]3O[C@H](O[C@@H]1CO)[C@H](,x,N,n',)[C@@H]
(O)[C@@H]1O[C@H](O[C@H](CO)[C@H]2O)[C@H](,x,N,n',)[C@H]2O,x
raffin|melit|melitri sugar disugar
OC[C@H]1OC(OC[C@H]2OC(O[C@@H]3(CO)[C@@H](O)[C@H](O)[C@@H](CO)O3)[C@H](O)[C@@H](O)
[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1O,x
gentiobi sugar disugar
O[C@H]1[C@H](OC[C@H]([C@@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@@H](O)[C@@H]
10,x
palatin sugar disugar
OC[C@@H]1(O)O[C@H](CO[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)[C@@H](O)[C@@H]
10,x
turan sugar disugar
O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1C(O)(CO)OC[C@@H](O)[C@H]1O,x
ose endersugar ose x,x
itol endersugar itol x,x
ityl endersugar makefree x,x
ide|id|oside|osid endersugar oside x,x
on|ono endersugar on x,x
uron|urono endersugar uron x,x
ar|aro endersugar ar x,x
odialdo|odiald endersugar dialdo x,x
oxirose|oxiros pyranose unknown 2,x
oxetose|oxetos pyranose unknown 3,x
furanose|furanos|ofuranose|ofuranos pyranose unknown 4,x
pyranose|pyranos|opyranose|opyranos pyranose unknown 5,x
septanose|septanos|oseptanose|oseptanos pyranose unknown 6,x
tetro multisugar unknown 4,x
pento multisugar unknown 5,x
hexo multisugar unknown 6,x
hepto multisugar unknown 7,x
octo multisugar unknown 8,x
nono multisugar unknown 9,x
deco multisugar unknown 10,x
ulo|ul structsgugarender ulose C=O,x
osamine structsgugarender osamine N,x
deoxy|desoxy deoxy unknown C,x

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inositol pseudosugar unknown x,x
 inositol root root OC1C(O)C(O)C(O)C(O)C1O,x
 mesoinositol|myoinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),
 x,[C@@H],6, Ring, Ring1, O,x
 scylloinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),x
 ,[C@@H],6, Ring, Ring1, O,x
 epiinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@@H],2,(O),x,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@@H],5,(O)
 ,x,[C@@H],6, Ring, Ring1, O,x
 dinositol root root O[C@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1O,x
 linositol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](O)[C@H](O)[C@H]1O,x
 quebrachitol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](OC)[C@H](O)[C@H]1O,x
 muram pseudosugar unknown x,x
 muram root root
 CC(C)O,x,[C@H],3, Ring, Ring1, [C@H],4,(O),x,[C@@H],5,(,x,C,6,O,x,) ,x,O,x,[C@H],1,(
 O),x,[C@H],2,(,x,N,n,) ,x, Ring, Ring1
 neuramin pseudosugar unknown x,x
 neuramin root root
 C,x,[C@@],2, Ring, Ring1, (O),x,O,x,[C@@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x,) ,x,[C@H],5,(,x,N,n,) ,x,[C@@H],4,(O),x,C,3, Ring, Ring1
 sial pseudosugar unknown x,x
 sial root root
 C,x,[C@@],2, Ring, Ring1, (O),x,O,x,[C@@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x,) ,x,[C@H],5,(,x,NC(=O)C,x,) ,x,[C@@H],4,(O),x,C,3, Ring, Ring1

 adenos|adenyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(,x,N,n|n6,) ,x,n,1,c,2,n,3
 ,c,4, Ring, Ring3, Ring, Ring2
 cytid|cytidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3,c,4,(,x,N,n|n4,) ,x,c,5,c,6, Ring, Ring2
 guanos|guanyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(=O),x,N,1,c,2,(,x,N,n|n2,
) ,x,n,3,c,4, Ring, Ring3, Ring, Ring2
 inos nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(O),x,n,1,c,2,n,3,c,4, Ring
 , Ring3, Ring, Ring2
 thymid|thymidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,C,2', [C@@H],1', (O,x, Ring, Ring1,) ,x
 ,n,1, Ring, Ring2, c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,(C),x,c,6, Ring, Ring2
 urid|uridyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,c,6, Ring, Ring2
 xanthos|xanthoyl|xanthonyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(O),x,n,1,c,2,(O),x,n,3,c,
 4, Ring, Ring3, Ring, Ring2
 orotid|orotidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3,c,4,(=O),x,c,5,c,6,(C(=O)O),x, Ring, Rin
 g2

cordycep nucleotide nucleotide

O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6, (x,N,n|n6,),x,n,1,c,2,n,3,c,4, Ring, Ring3, Ring, Ring2

adenyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6, (x,N,n|n6,),x,n,1,c,2,n,3,c,4, Ring, Ring3, Ring, Ring2

cytidyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,1, Ring, Ring2, c,2, (=O),x,n,3,c,4, (x,N,n,),x,c,5,c,6, Ring, Ring2

guanyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6, (=O),x,n,1,c,2, (x,N,n|n2,),n,3,c,4, Ring, Ring3, Ring, Ring2

inos loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6, (O),x,n,1,c,2,n,3,c,4, Ring, Ring3, Ring, Ring2

thymidyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x,C,2', [C@H],1', (O,x, Ring, Ring1,),x,n,1, Ring, Ring2, c,2, (=O),x,n,3|n,c,4, (=O),x,c,5, (C),x,c,6, Ring, Ring2

uridyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,1, Ring, Ring2, c,2, (=O),x,n,3|n,c,4, (=O),x,c,5,c,6, Ring, Ring2

xanthoyl|xanthonyl loveracid root

P,x, (=O),x, (x,O,1@o'),x, (x,O,1@o'),x,O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6, (O),x,n,1,c,2, (O),x,n,3,c,4, Ring, Ring3, Ring, Ring2

purineriboside root root

O,x,C,5', [C@H],4', Ring, Ring1, [C@H],3', (O),x, [C@H],2', (O),x, [C@H],1', (O,x, Ring, Ring1,),x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,n,1,c,2,n,3,c,4, Ring, Ring3, Ring, Ring2

thuj root root

C,3, Ring, Ring1, C,2,C,1, Ring, Ring2, (x,C,7, (x,C,8,),x,C,9,),x,C,6,C,5, Ring, Ring2, C,4, Ring, Ring1, (x,C,10,),x

car root root

C,1, Ring, Ring1, Ring, Ring2, C,2,C,3, (x,C,4,C,5,C,6, Ring, Ring1, (x,C,7, Ring, Ring2, (x,C,8,),x,C,9,),x,),x,C,10

norcar root root

C,1, Ring, Ring1, Ring, Ring2, C,2,C,3,C,4,C,5,C,6, Ring, Ring1, (x,C,7, Ring, Ring2,),x

pin root root

C,2, Ring, Ring1, (x,C,10,),x,C,3,C,4,C,5, (x,C,7, Ring, Ring2,),x,C,6, (x,C,8,) (x,C,9,),x,C,1, Ring, Ring2, Ring, Ring1

norpin root root

C,2, Ring, Ring1, C,3,C,4,C,5, (x,C,7, Ring, Ring2,),x,C,6,C,1, Ring, Ring2, Ring, Ring1

camphor loveracid root

C,10,C,1, Ring, Ring1, Ring, Ring2, C,2,C,3,C,4, (x,C,5,C,6, Ring, Ring1,),x,C,7, (x,C,8,),x, (x,C,9,),x, Ring, Ring2

camphor root root

C,10,C,1, Ring, Ring1, Ring, Ring2, C,2, (=O),x,C,3,C,4, (x,C,5,C,6, Ring, Ring1,),x,C,7, (x,C,8,),x, (x,C,9,),x, Ring, Ring2

norcamphor root root
C,1, Ring, Ring1, Ring, Ring2, C,2, (=O), x, C,3, C,4, (, x, C,5, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
camphorquinone|camphoroquinone root root
C,10, C,1, Ring, Ring1, Ring, Ring2, C,2, (=O), x, C,3, (=O), x, C,4, (, x, C,5, C,6, Ring, Ring1,), x, C,7, (, x, C,8,), x, (, x, C,9,), x, Ring, Ring2
borne|born|camphane|camphan|bornylane|bornylan|isoborne|isoborn root root
C,2, Ring, Ring1, C,3, C,4, Ring, Ring2, C,5, C,6, C,1, Ring, Ring1, (, x, C,7, Ring, Ring2, (, x, C,8,), x, C,9,), x, C,10
camphan loveracid root
C,1, Ring, Ring1, Ring, Ring2, O,2, C,3, (=O), x, C,4, (, x, C,5, C,6, Ring, Ring1,), x, (, x, C,7, (, x, C,x,) (, x, C,x,) x, Ring, Ring2,), x, C,x
norborne|norborn|norborna root root
C,1, Ring, Ring1, Ring, Ring2, C,2, C,3, C,4, (, x, C,5, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
norbornadien|norbornadiene|25norbornadien|25norbornadiene root root
C,1, Ring, Ring1, Ring, Ring2, C,2, =, x, C,3, C,4, (, x, C,5, =, x, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
norbornen|norbornene|2norbornen|2norbornene root root
C,1, Ring, Ring1, Ring, Ring2, C,2, =, x, C,3, C,4, (, x, C,5, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
5norbornen|5norbornene root root
C,1, Ring, Ring1, Ring, Ring2, C,2, C,3, C,4, (, x, C,5, =, x, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
camphene|camphen root root
C,1, Ring, Ring1, Ring, Ring2, C,2, (, x, C,x,), x, (, x, C,x,), x, C,3, (, x, =, x, C,x,), x, C,4, (, x, C,5, C,6, Ring, Ring1,), x, C,7, Ring, Ring2
phosgene|phosgen root root ClC(=O)Cl,x
triphosgene|triphosgen root root C(Cl)(Cl)(Cl)OC(=O)OC(Cl)(Cl)(Cl),x
glyoxyl root root C,1,C,2|w|omega,=,x,O,x
pyruv root root C,1,C,2,(=,x,O,x,),x,C,3|w|omega
glycerol|snglycerol|racglycerol pseudosugar unknown x,x
glycerol|snglycerol|snglycero|racglycerol|racglycero|glycero|glycerine root root
O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma
glycerin root root O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma
glycerone|glyceron root root O,1@1|a|alpha,C,x,C,x,(=O),x,C,x,O,1@3|g|gamma
in|anoin glycerin root
O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma|a'|alpha'
gerani|geran root root
C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,/,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
tetrahydrogerani|geran root root
C,1,C,2,C,3,(,x,C,x,),x,C,4,C,5,C,6,C,7,(,x,C,x,),x,C,8
ner root root
C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,\,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
phyt root root
C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x
citral root root
O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x
ethylcitral root root
O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x
citronell|betacitronell|baran root root CCC(C)CCC=C(C)C,x
linalo root root C(CCC=C(C)C)(C=C)C,x
dihydrolinalo root root C(CCC=C(C)C)(CC)C,x
tetrahydrolinalo root root C(CCCC(C)C)(CC)C,x
lavandul root root CC(C(=C)C)CC=C(C)C,x
tetrahydrolavandul root root CC(C(C)C)CCC(C)C,x

farnes root root
C,1,C,2,=,x,C,3,(C),x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8,C,9,C,10,=,x,C,11,(C)C,x
ocimene root root C,1,=,x,C,2,C,3,(C)=,x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8
alloocimene|allocimen root root
C,1,C,2,(C)=,x,C,3,C,4,=,x,C,5,(C),x,C,6,=,x,C,7,C,8
nerolid root root C(C)(C=C)CCC=C(C)CCC=C(C)C,x
all root root C,1|a|alpha,C,2|b|beta,=,x,C,3|g|gamma
isoall root root C,1|a|alpha,=,x,C,2|b|beta,C,3|g|gamma
homoall root root C,1|a|alpha,C,2|b|beta,C,3|g|gamma,=,x,C,4|d|delta
methall root root C,1,C,2,(x,C,x),x,=,x,C,3
triazeno root root N,4@1,=,x,N,2,N,3
vin root root C,1|a|alpha,=,x,C,2|b|beta
hydrazine|hydrazin root root N,1|n,N,2|n'
dithioiminocarbonate root root S,1@s,C,x,(=,x,N,n),x,S,1@s'
urea|carbamide|carbamid root root N,1|n,C,2,(x,=,x,O,o),x,N,3|n'
sulfocarbamide|sulfocarbamid|sulfourea root root
N,1|n,C,2,(x,=,x,S,s),x,N,3|n'
biurea root root N,1,C,2,(=O),x,N,3,N,4,C,5,(=O),x,N,6
guanyl root root C,4@x,(=N),x,N,x
uronium root root N,1|n,C,2,(x,N,3|n'),x,=,x,[O+],o
ureido root root N,4@1|n,C,2,(x,=,x,O,o),x,N,3|n'
ureylene|ureylen root bridge N,4@1|n,C,2,(x,=,x,O,o),x,N,4@3|n'
carbanilide|carbanilid root root
c,6,ring,ring1,c,5,c,4,c,3,c,2,c,1,ring,ring1,N,n,C,x,(x,=,x,O,o),x,N,n',c,1',
ring,ring2,c,2',c,3',c,4',c,5',c,6',ring,ring2
tms root root [Si],4@x,(C)(C)(C),x
tbdms root root [Si],4@x,(C(C)(C)C)(C)(C),x
plumb root root [Pb],1
sil root root [Si],x
stann root root [Sn],x
bor root root [B],x
germ root root [Ge],x
amine|amin|ammonia root root N,n
phosphine|phosphin root root P,x
arsine|arsin root root [As],x
hydrogen root root [H],4@x
deuterium root root [2H],4@x
tritium root root [3H],4@x
hydrido root root [H-],4@x
deuterido root root [2H-],4@x
lithio root root [Li],4@x
sodio root root [Na],4@x
potassio|kalio root root [K],4@x
fluoro|fluor root root F,4@x
chloro|chlor root root Cl,4@x
chlorosyl root root Cl,4@x,=O,x
chloryl root root Cl,4@x,(=O)=O,x
perchloryl root root Cl,4@x,(=O)(=O)=O,x
borono root root [B],4@x,(O)O,x
lithium root metal [Li],x
sodium|natrium root metal [Na],x
potassium|kalium root metal [K],x
rubidium root metal [Rb],x
cesium root metal [Cs],x
francium root metal [Fr],x
beryllium|glucinium root metal [Be],x
magnesium root metal [Mg],x

copper root metal [Cu],x
silver|argent root metal [Ag],x
gold root metal [Au],x
zinc root metal [Zn],x
cadmium root metal [Cd],x
mercury root metal [Hg],w
boron root nonmetal [B],x
aluminum|alane root metal [Al],x
gallium root metal [Ga],x
indium root metal [In],x
thallium root metal [Tl],x
carbon root nonmetal [C],x
silicon root nonmetal [Si],x
germanium root metal [Ge],x
tin root metal [Sn],x
lead root metal [Pb],x
nitrogen root nonmetal [N],x
phosphorus root nonmetal [P],x
arsenic root nonmetal [As],x
antimony|stibium root metal [Sb],x
bismuth root metal [Bi],x
oxygen root nonmetal [O],x
sulfur root nonmetal [S],x
selenium root nonmetal [Se],x
tellurium root nonmetal [Te],x
polonium nonroot metal [Po],x
fluorine root nonmetal [F],x
chlorine root nonmetal [Cl],x
bromine root nonmetal [Br],x
iodine root nonmetal [I],x
astatine root nonmetal [At],x
helium root nonmetal [He],x
neon root nonmetal [Ne],x
argon root nonmetal [Ar],x
krypton root nonmetal [Kr],x
xenon root nonmetal [Xe],x
radon root nonmetal [Rn],x

bromo|brom root root Br,4@x
iodo|iod root root I,4@x
iodosyl|iodoso root root I,4@x,=O,x
iodyl|iodoxy root root I,4@x,(=O)=O,x
deutero|deuterio root root [2H],4@x
nitro root root [N+],4@x,(=O)[O-],x
acinitro root root [N+],8@x,(O)[O-],x
nitroso|nitros|nitrosyl root root N=O,4@x
nitrosamido root root N,4@x,N=O,x
nitrosamide root root NN=O,x
nitrosonium root root [NH0+],x,=O,x
isonitroso|isonitros root root N,8@x,O,x
hydroxy|hydroxo root root O,4@x
hydroxyl root root O,4@o
hydroselene root root [Se],4@x
hydrotelluro root root [Te],4@x
cyano|cyanogen root root C#N,4@x
isocyano|isonitrilo root root [N+]#[C-],4@x
cyanato root root OC#N,4@x

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isocyanato root root N=C=O,4@x
thiocyanato root root SC#N,4@x
isothiocyanato root root N=C=S,4@x
selenocyanato root root [Se]C#N,4@x
isoselenocyanato root root N=C=[Se],4@x
diazoo root root [N+],8@x,[N-],x
diazoate|diazoat root root [N+],8@x,=N,x,[O-],x
azido|triazoo root root N,4@x,[N+]=[N-],x
oxo|keto root root O,8@x
oxido root root [O-],4@x
thioxo|thiono root root S,8@x
sulfido root root [S-],4@x
selenoxo root root [Se],8@x
telluroxo root root [Te],8@x
mercapto root root S,4@x
hydroperoxy root root O,4@x,O,x
carboxy root root C,4@x,(=,x,O,x),x,O,x
amidino root root C,4@x,(x,N,x)=,x,N,x
aminoiminometh root root C,x,(=,x,N,x),x,N,x
sulfo root heterolover S,4@x,(=O),x,(=O),x,O,x
sulfoxy root root O,4@x,S,x,(=O),x,(=O),x,O,x
sulfoamido root root N,4@x,S,x,(=O),x,(=O),x,O,x
sulfino root root S,4@x,(=O),x,O,x
sulfeno root root S,4@x,O,x
sulfonato root root S,4@x,(=O),x,(=O),x,[O-],x
phosphonato|phosphato root root P,4@x,(=O),x,([O-]),x,[O-],x
hydrogenphosphato root root P,4@x,(=O),x,(O),x,[O-],x
dihydrogenphosphato root root P,4@x,(=O),x,(O),x,O,x
phosphinato root root P,4@x,(=O),x,[O-],x
phosphono|phosphoro infix infix P,4@x,(=O),x,(x,O,1@o'),x,O,1@o
phospho root heterolover P,4@x,(=O),x,(O),1@x,O,1@x
diphospho root heterolover P,4@x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,1@x
triphospho root heterolover
P,4@x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,1@x
phosphinico root root P,8@x,(=O),x,O,1@o
arsonato root root [As],4@x,(=O),x,([O-]),x,[O-],x
arsinato root root [As],4@x,(=O),x,[O-],x
arsono|arsoro root root [As],4@x,(=O),x,(x,O,1@o'),x,O,1@o
arsinico root root [As],8@x,(=O),x,O,1@o
mesyl root root S,4@x,(=O),x,(=O),x,C,x
-part2-toluene root root C,4@a|alpha
-part2-cumene root root C,4@7|a|alpha,(x,C,8|b|beta),x,C,9
-part2-cymene root root C,4@8|a|alpha,(x,C,9),x,C,10
-part2-anisidine root root O,4@x,C,a|alpha
-part2-thioanisidine root root S,4@x,C,a|alpha
-part2-phenetidine root root O,4@x,C,a|alpha,C,b|beta
-part2-xylylidine root root C,4@a|alpha
-part2-arsanil root root N,4@n
-part2-coumar root root O,4@x
indophenol root root
O,x,=,x,C,1, Ring, Ring1, C,2,=,x,C,3,C,4,(x,C,5,=,x,C,6, Ring, Ring1),x,=,x,N,x,C,
1', Ring, Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,=,x,C,4',(x,O,x),x,C,5',=,x,C,6', Ri
ng, Ring2
thymolindophenol root root
O,x,=,x,C,1, Ring, Ring1, C,2,=,x,C,3,C,4,(x,C,5,=,x,C,6, Ring, Ring1),x,=,x,N,x,C,
1', Ring, Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,(x,C,x,(x,C,x),x,C,x),x,=,x,C,4',
(x,O,x),x,C,5',=,x,C,6',(x,C,x),x, Ring, Ring2

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cresolindphenol root root
O,x,=,x,C,1, Ring, Ring1, C,2,=,x,C,3,C,4, (,x,C,5,=,x,C,6, Ring, Ring1,),x,=,x,N,x,C,1', Ring, Ring2, =,x,C,2' |m| meta, (C), x,C,3' |o| ortho, =,x,C,4', (,x,O,x,), x,C,5', =,x,C,6', Ring, Ring2
picoline|picolin|picol toluene picoline
c,2, Ring, Ring1, c,3 |b| beta, c,4 |g| gamma, c,5, c,6, n,1, Ring, Ring1
pipecoline|pipecolin|pipecol toluene picoline
C,2 |a| alpha, Ring, Ring1, C,3 |b| beta, C,4 |g| gamma |p, C,5, C,6, N,1, Ring, Ring1
toluene|tolu|tol toluene toluene
c,1, Ring, Ring1, c,2 |o| ortho, Ring, Ring2, ., x, c,4 |p| para, Ring, Ring3, Ring, Ring4, ., x, c,6, Ring, Ring5, Ring, Ring1, ., x, c,3 |m| meta, Ring, Ring2, Ring, Ring3, ., x, c,5, Ring, Ring4, Ring, Ring5
toluidide|otoluidide|toluide|otoluide toluidide toluene
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', Ring, Ring1
cumidine|cumidin toluene cumene
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cumene|cumen toluene cumene
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cumyl|alphacumyl root root
C,4@a|alpha, (C) (C), x, c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, Ring, Ring1
cumidene|cumiden toluene cumene
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cymene|cymen toluene cymene
C,7 |a| alpha, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xylene|xylol toluene toluene
C,a|alpha, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xylen|xyl toluene xyloidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xyloidide|oxyloidide|xyloide|oxyloide toluidide xyloidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', Ring, Ring1
anis toluene anisidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
thioanis toluene thioanisidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
homoanis toluene anisidine
C,x,C,x, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
anisidide|oanisidide|aniseide|oaniseide toluidide anisidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', Ring, Ring1
anisal toluene anisidine
C,8@x, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
mentha|menth|neomenth|neomentha|isomenth|isomentha toluene cymene
C,3 |m| meta, Ring, Ring1, C,4 |p| para, C,5, C,6, C,1, Ring, Ring2, C,2 |o| ortho, Ring, Ring1, ., x, C,7 |a| alpha, Ring, Ring2
anisidine|anisidin toluene anisidine
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
anisidino toluene anisidine
N,4@n, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
phenetidine|phenetidin toluene phenetidine
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
phenetidide|ophenetidide|phenetide|ophenetide toluidide phenetidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', Ring, Ring1
phenetidino toluene phenetidine
N,4@n, c,1, Ring, Ring1, c,2 |c| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1

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cresyl toluene toluene
O,x,c,1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, =, x, c, 6, Ring, Ring1
cres toluene toluene
c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
thiocresol toluene toluene
S, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
cresylicacid toluene toluene
O, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
cresot toluene toluene
c, 2, Ring, Ring1, (O), x, c, 3 | o | ortho, c, 4 | m | meta, c, 5 | p | para, c, 6, c, 1, (, x, C, x, ), x, Ring,
Ring1
toluidine|toluidin toluene toluene
N, n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
toluidino toluene toluene
N, 4@n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
xylidine|xylidin toluene xyloidine
N, n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
xyloidino toluene xyloidine
N, 4@n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
coumar toluene coumar
C, x, C, a | alpha, =, x, C, b | beta, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5,
c, 6, Ring, Ring1
arsanil toluene tolarsanil
[As], x, (, x, O, 1@x, ), x, (, x, O, 1@x, ), x, (=O), x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta,
c, 4 | p | para, c, 5, c, 6, Ring, Ring1
tosyl|ptosyl root root
S, 4@x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc, x, (, x, C, x, ), x, cc, x, Ring, Ring1
tosylate|ptosylate|tosylat|ptosylat|tosilate|ptosilate|tosilat|ptosilat root
root O, 1@x, S, x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(C)cc, x, Ring, Ring1
tosylamido root root
N, 4@x, S, x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(C)cc, x, Ring, Ring1
brosylate|brosylat|brosilate|brosilat root root
O, 1@x, S, x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(Br)cc, x, Ring, Ring1
brosyl root root S, 4@x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(Br)cc, x, Ring, Ring1
closylate|closylat|closilate|closilat root root
O, 1@x, S, x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(Cl)cc, x, Ring, Ring1
closyl root root S, 4@x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(Cl)cc, x, Ring, Ring1
nosylate|nosylat|nosilate|nosilat root root
O, 1@x, S, x, (=O), x, (=O), x, c, x, Ring, Ring1, cc([N+](=O)[O-])ccc, x, Ring, Ring1
mesylate|mesylat root root O, 1@x, S, x, (=O), x, (=O), x, C, x
esylate|esylat root root O, 1@x, S, x, (=O), x, (=O), x, C, x, C, x
pipsyl root root S, 4@x, (=O), x, (=O), x, c, x, Ring, Ring1, ccc(I)cc, x, Ring, Ring1
methosulfate|methosulfat|metilsulfate|metilsulfat root root
O, 1@x, S, x, (=O), x, (=O), x, O, x, C, x
ethosulfate|ethosulfat|etilsulfate|etilsulfat root root
O, 1@x, S, x, (=O), x, (=O), x, O, x, C, x, C, x
desyl root root C, x, (C(=O)clcccccl)c2cccc2, x
isoniazide|isoniazid root root
c, 2, Ring, Ring1, c, 3, c, 4, (, x, C, x, (, x, =, x, O, x, ), x, N, x, N, n, ), x, c, 5, c, 6, n, 1, Ring, Ring
1
pheneth root root
C, a | alpha, C, b | beta, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring,
Ring1
secpheneth root root
C, a | alpha, (, x, C, b | beta, ), x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5,
c, 6, Ring, Ring1

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neoph root root
C,a|alpha,C,b|beta,(C)(C),x,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5
,c,6, Ring, Ring1
amphetamine|amphetamin root root
N,n,C,a|alpha,(C),x,C,b|beta,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
5,c,6, Ring, Ring1
methamphetamine|methamphetamin root root
C,x,N,n,C,a|alpha,(C),x,C,b|beta,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|par
a,c,5,c,6, Ring, Ring1
ammelide root root
N,n,c,6, Ring, Ring1, n,1,c,2,(,x,O,x,),x,n,3,c,4,(,x,O,x,),x,n,5, Ring, Ring1
phenate|phenat|phenoxide|phenoxid root root [O-
],x,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Ring, Ring1
phen root phenyl
c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Ring, Ring1
benzyne|benzyn root root
C,1, Ring, Ring1, #,x,C,2|o|ortho,C,3|m|meta,=,x,C,4|p|para,C,5,=,x,C,6, Ring, Ring1
benzal root root
C,8@a|alpha,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Ring, Ring1
benzene|benzen|benzol root root
c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Ring, Ring1
dewarbenzene root root C12C=CC1C=C2,x
benzeneoxid|benzeneoxide root root
C,1, Ring, Ring1, (,x,O,x, Ring, Ring2, ),x,C,2, Ring, Ring2, C,3,=,x,C,4,C,5,=,x,C,6, Rin
g, Ring1
benzo-quinone|benzo-quinon root root
C,1, Ring, Ring1, (=O),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x,C,6,R
ing, Ring1
benzo-quinodimethane|benzo-quinodimethan root root
C,1, Ring, Ring1, (=,x,C,2@7, ),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=,x,C,2@8, )
,x,C,5,=,x,C,6, Ring, Ring1
toluquinone|ptoluquinone root root
C,1, Ring, Ring1, (=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
,C,6, Ring, Ring1
xyloquinone|pxyloquinone root root
C,1, Ring, Ring1, (=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
,C,6,(C),x, Ring, Ring1
duroquinone root root CC(C(C(C)=C1C)=O)=C(C1=O)C,x
thymoquinone root root O=C(C(C)=C1)C=C(C1=O)C(C)C,x
hemellitot root root
c,1,(C),x, Ring, Ring1, c,2|o|ortho,(C),x,c,3|m|meta,(C),x,c,4|p|para,c,5,c,6, Ring,
Ring1
benzo|benz benzo benzo
c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Ring, Ring1
acene|acen acene acene c1ccccc1,x
aphene acene aphene c1ccccc1,x
mandel|amygdal root root
C,x,C,x,(,x,O,x, ),x,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6, Rin
g, Ring1
mesit root root
c,2|o|ortho, Ring, Ring1, c,3|m|meta,(,x,C,alpha1|alpha2|alpha, ),x,c,4|p|para,c,5,(
,x,C,alpha3|alpha4|alpha', ),x,c,6,c,1,(,x,C,alpha5|alpha6|alpha'', ),x, Ring, Ring1
mesitylene|mesitylen root root
C,alpha1|alpha2|alpha,c,1, Ring, Ring1, c,2|o|ortho,c,3|m|meta,(,x,C,alpha3|alpha4|
alpha', ),x,c,4|p|para,c,5,(,x,C,alpha5|alpha6|alpha'', ),x,c,6, Ring, Ring1
durene|duren root root
C,a|alpha|alpha1,c,1, Ring, Ring1, c,2|o|ortho,(,x,C,a'|alpha'|alpha2, ),x,c,3|m|met

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a,c,4|p|para,(,x,C,a''|alpha''|alpha4,),x,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
,Ring,Ring1
isodurene|isoduren root root
C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met
a,(,x,C,a''|alpha''|alpha3,),x,c,4|p|para,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
,Ring,Ring1
anisole|anisol root root
C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
1
catechol root root
c,1,Ring,Ring1,(,x,O,o,),x,c,2|ortho,(,x,O,o',),x,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring,Ring1
phenetole|phenetol root root
C,b|beta,C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring,Ring1
anethole|anethol root root
C,x,O,x,c,1,Ring,Ring1,c,2 o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x,C,x,),x
,c,5,c,6,Ring,Ring1
dihydroanethole|dihydroanethol root root
C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x,),x,c,5
,c,6,Ring,Ring1
guaiacol root root
C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,Rin
g,Ring1
guaiacolate root root
C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,1@x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,R
ing,Ring1
veratrole|veratrol root root
C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
eugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,=,x
,C,x,),x,c,5,c,6,Ring,Ring1
dihydroeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x
,),x,c,5,c,6,Ring,Ring1
isoeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x
,C,x,),x,c,5,c,6,Ring,Ring1
isoeugenol root root
O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,=,x
,C,x,C,x,),x,c,5,c,6,Ring,Ring1
styr|styrene|styren|styrol|cinnamene|cinnamenol|cinnamol root root
C,b|beta|w|omega,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,
c,5,c,6,Ring,Ring1
styrall|styral root root
C,b|beta,(,x,C,a|alpha,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c,6,Ring,Ring1
phosphinine root root
p,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anthranil root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,(,x,N,n,),x,c,3|m|meta,c,4|p|para,c,5,c,6,R
ing,Ring1
hippur root trivial
C,x,C,x,N,x,C,x,(,x,=,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para
,c,5,c,6,Ring,Ring1

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carbanil loveracid root
C,x,N,x,c,1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
shikim root root
C,x,C,1, Ring, Ring1, =, x, C, 2, C, 3, (O), x, C, 4, (O), x, C, 5, (O), x, C, 6, Ring, Ring1
benzo|benz|dracyl root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
crithmin root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (C), x, c, 5, c, 6, Ring, Ri
ng1
dracon root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, R
ing1
vanill root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, ), x, c, 4 | p | para, (, x, O
, x, ), x, c, 5, c, 6, Ring, Ring1
isovanill root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (O), x, c, 4 | p | para, (OC), x, c, 5, c, 6,
Ring, Ring1
homovanill root root
C,a|alpha, C, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, ), x, c, 4 | p | para, (
, x, O, x, ), x, c, 5, c, 6, Ring, Ring1
vanillin root root
O, x, Ring, Ring2, ., x, O, x, =, x, C, a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (OC),
x, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
ethylvanillin root root
O, x, Ring, Ring2, ., x, O, x, =, x, C, a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (OCC)
, x, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
isovanillin root root
O, x, Ring, Ring2, ., x, O, x, =, x, C, a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, Ring,
Ring2, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring1
acetovanillone root root
O, x, =, x, C, a|alpha, (C), x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, ), x, c,
4 | p | para, (, x, O, x, ), x, c, 5, c, 6, Ring, Ring1
safrole|safrol root root
C, x, =, x, C, x, C, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, O, x, Ring, Ring2
, ), x, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
dihydrosafrole|dihydrosafrol root root
C, x, C, x, C, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, O, x, Ring, Ring2, ), x
, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
isosafrole|isosaflol root root
C, x, C, x, =, x, C, x, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, O, x, Ring, Ring2
, ), x, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
piperon root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, O, x, Ring, Ring2, ), x, c
, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
homopiperon root root
C,a|alpha, C, b|beta, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, C, x, O, x, Ring, Ri
ng2, ), x, c, 4 | p | para, Ring, Ring2, c, 5, c, 6, Ring, Ring1
veratr root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (OC), x, c, 4 | p | para, (OC), x, c, 5, c, 6
, Ring, Ring1
homoveratr root root
C,a|alpha, C, b|beta, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (OC), x, c, 4 | p | para, (OC),
x, c, 5, c, 6, Ring, Ring1
protocatechu root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, (, x, O, x, ), x, c, 4 | p | para, (, x, O, x,
), x, c, 5, c, 6, Ring, Ring1

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homoprotocatechu root root
C,a|alpha,C,b|beta,c,1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, (, x, O, x,) , x, c, 4 |p|para, (, x, O, x,) , x, c, 5, c, 6, Ring, Ring1
citrazin root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, (, x, O, x,) , x, n, 4 |p|para, c, 5, (, x, O, x,) , x, c, 6, Ring, Ring1
gall root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, (, x, O, x,) , x, c, 4 |p|para, (, x, O, x,) , x, c, 5, (, x, O, x,) , x, c, 6, Ring, Ring1
gallacetophenone root root O=C(C)C1=C(O)C(O)=C(O)C=C1,x
toluene|toluol root root
C,a|alpha, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, =, x, c, 6, Ring, Ring1
1
cumene|cumen root root
C,x,C,a|alpha, (, x, C, x,) , x, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
aniline|anilin|aniline|anilin root root
N,n,c,1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
anilino|analino root root
N,4@n,c,1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
gentis root root
C,x,c,1, Ring, Ring1, c, 2, (, x, O, o,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, (, x, O, o',) , x, c, 6, Ring, Ring1
homogentis root root
C,x,C,x,c,1, Ring, Ring1, c, 2, (, x, O, o,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, (, x, O, o',) , x, c, 6, Ring, Ring1
salicyl|salic root root
C,x,c,1, Ring, Ring1, c, 2, (, x, O, o,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
salicylal root root
C,8@x,c,1, Ring, Ring1, c, 2, (, x, O, o,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
anilot root root
C,x,c,1, Ring, Ring1, c, 2, (, x, O, o,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, ([N+] (=O) [O-]) , x, c, 6, Ring, Ring1
alpharesorcy|aresorcy root root
C,x,c,1, Ring, Ring1, c, 2, c, 3 |m|meta, (, x, O, x,) , x, c, 4 |p|para, c, 5, (, x, O, x,) , x, c, 6, Ring, Ring1
betaresorcy|bresorcy root root
C,x,c,1, Ring, Ring1, c, 2, (, x, O, x,) , x, c, 3 |m|meta, c, 4 |p|para, (, x, O, x,) , x, c, 5, c, 6, Ring, Ring1
gammaresorcy|gresorcy root root
C,x,c,1, Ring, Ring1, c, 2, (, x, O, x,) , x, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, (, x, O, x,) , x, Ring, Ring1
phenac root root
C,a|alpha,C,x, (, x, =, x, O, x,) , x, c, x, Ring, Ring1, =, x, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
trop root root
C,x,C,x, (, x, C, x, O, x,) , x, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
nortrop root root
C,x, (, x, C, x, O, x,) , x, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
hydratrop root root
C,x,C,x, (, x, C, x,) , x, c, 1, Ring, Ring1, c, 2 |o|ortho, c, 3 |m|meta, c, 4 |p|para, c, 5, c, 6, Ring, Ring1
homatrop root root CN1C2CCC1CC(OC(C(O)C3=CC=CC=C3)=O)C2,x
atrop root root OCC(C(OC3CC2CCC(C3)N2C)=O)c1cccc1,x

[illegible]

naphtho-quinone|naphtho-quinon|naphthalene-quinone|naphthalene-quinon root root
 c,1|a|alpha,(=O),x,Ring,Ring1,c,2|b|beta,=,x,c,3,c,4,(=O),x,c,4a|4alpha,Ring,Rin
 g2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
 cadalene|cadalen root root
 c,1|a|alpha,(C),x,Ring,Ring1,c,2|b|beta,c,3,c,4,(C(C)C),x,c,4a|4alpha,Ring,Ring2
 ,c,5,c,6,(C),x,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
 benzodioxene|benzodioxen root root
 o,1,Ring,Ring1,c,2,c,3,o,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ri
 ng,Ring1,Ring,Ring2
 azulene|azulen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
 Ring2
 azuleno|azulen opfuser unknown
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
 Ring2
 anthracene|anthracen|anthro|anthr root root
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Rin
 g3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
 anthrone|anthron root root
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a,Ring,Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,(=,x,O,x,),x,c,9a,Ring,Ring2,Ring,Ring1
 anthra-quinone|anthra-quinon|anthracene-quinone|anthracene-quinon root root
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,(=O),x,c,5a|10a,R
 ing,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,(=,x,O,x,),x,c,9a,Ring,Ring2,Ring,
 Ring1
 anthra|anthraceno opfuser unknown
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Rin
 g3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
 acrid root root
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
 aminacrine|aminacrin|aminacridin|aminacridine|monacrin|monacrine root root
 c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
 ,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,(N),n,c,9a,Ring,Ring2,Ring,Ring1
 acenaphthene|acenaphthen root root
 C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
 Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
 acenaphtho|acenaphth opfuser unknown
 C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
 Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
 acenaphthylene|acenaphthylen root root
 c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
 Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
 cholanthrene|cholanthren root root
 C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
 g4,c,6b,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,12,c,12a,Ring,Ring4,
 c,12b,Ring,Ring1,c,12c,Ring,Ring3,Ring,Ring2
 phenalene|phenalen root root
 c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
 ,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3
 julolid root root
 C,1,Ring,Ring1,C,2,c,C,N,4,Ring,Ring2,C,5,C,6,C,7,c,7a,Ring,Ring3,c,8,c,9,c,10,c
 ,10a,Ring,Ring1,c,10b,Ring,Ring2,Ring,Ring3
 perimid root root
 n,1,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
 ,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3

phenanthren|phenanthrene root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a, Ring, Ring3, c,9, c,10, c,10a, Ring, Ring1, Ring, Ring2
phenanthr|phenanthro|phenanthra opfuser unknown
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a, Ring, Ring3, c,9, c,10, c,10a, Ring, Ring1, Ring, Ring2
cyclopentadefphenanthren|cyclopentadefphenanthrene root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,4a, Ring, Ring3, c,5, c,6, c,7, c,7a, Ring, Ring4, c,8, c,9, c,8a, Ring, Ring1, c,8b, Ring, Ring2, c,8c, Ring, Ring3, Ring, Ring4
bathophenanthroline root root
n,1, Ring, Ring1, c,2, c,3, c,4, (c4cccc4), x, c,4a, Ring, Ring2, c,5, c,6, c,6a, Ring, Ring3, c,7, (c5cccc5), x, c,8, c,9, n,10, c,10a, Ring, Ring3, c,10b, Ring, Ring1, Ring, Ring2
phenanthrone|phenanthron root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a, Ring, Ring3, C,9, (=O), x, C,10, c,10a, Ring, Ring1, Ring, Ring2
phenanthrene-quinone|phenanthrene-quinon root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a, Ring, Ring3, c,9, (=O), x, c,10, (=O), x, c,10a, Ring, Ring1, Ring, Ring2
cyclopentaaphenanthrene|cyclopentaaphenanthren root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,5, Ring, Ring2, c,6, c,7, c,8, Ring, Ring3, c,14, Ring, Ring4, c,15, c,16, c,17, c,13, Ring, Ring4, c,12, c,11, c,9, Ring, Ring3, c,10, Ring, Ring2, Ring, Ring1
fluoranthene|fluoranth|fluoranthen root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,6a, Ring, Ring3, c,6b, Ring, Ring4, c,7, c,8, c,9, c,10, c,10a, Ring, Ring4, c,10b, Ring, Ring1, c,10c, Ring, Ring2, Ring, Ring3
acephenanthrene|acephenanthren root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,5a, Ring, Ring3, c,6, c,6a, Ring, Ring4, c,7, c,8, c,9, c,10, c,10a, Ring, Ring4, c,10b, Ring, Ring1, c,10c, Ring, Ring2, Ring, Ring3
acephenanthrylene|acephenanthrylen root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,5a, Ring, Ring3, c,6, c,6a, Ring, Ring4, c,7, c,8, c,9, c,10, c,10a, Ring, Ring4, c,10b, Ring, Ring1, c,10c, Ring, Ring2, Ring, Ring3
aceanthrene|aceanthren root root
C,1, Ring, Ring1, C,2, c,2a, Ring, Ring2, c,3, c,4, c,5, c,5a, Ring, Ring3, c,6, c,6a, Ring, Ring4, c,7, c,8, c,9, c,10, c,10a, Ring, Ring4, c,10b, Ring, Ring1, c,10c, Ring, Ring2, Ring, Ring3
aceanthrylene|aceanthrylen root root
c,1, Ring, Ring1, c,2, c,2a, Ring, Ring2, c,3, c,4, c,5, c,5a, Ring, Ring3, c,6, c,6a, Ring, Ring4, c,7, c,8, c,9, c,10, c,10a, Ring, Ring4, c,10b, Ring, Ring1, c,10c, Ring, Ring2, Ring, Ring3
violanthrene|violanthren root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, C,5, c,5a, Ring, Ring3, c,6, c,7, c,7a, Ring, Ring4, c,7b, Ring, Ring5, c,8, c,9, c,9a, (, x, c,18f, Ring, Ring6, c,18e, Ring, Ring7, Ring, Ring5,), x, C,10, c,10a, Ring, Ring8, c,11, c,12, c,13, c,14, c,14a, Ring, Ring8, c,14b, Ring, Ring6, c,15, c,16, c,16a, Ring, Ring7, c,16b, Ring, Ring9, c,17, c,18, c,18a, (, x, c,18b, Ring, Ring1, Ring, Ring2,), x, c,18c, Ring, Ring3, c,18d, Ring, Ring4, Ring, Ring9
isoviolanthrene|isoviolanthren root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,6a, (, x, c,18c, Ring, Ring4, c,18b, Ring, Ring5, Ring, Ring3,), x, c,6b, Ring, Ring6, c,7, c,8, c,8a, (, x, c,18e, Ring, Ring7, c,18d, Ring, Ring8, Ring, Ring6,), x, C,9, c,9a, Ring, Ring9, c,10, c,11, c,12, c,13, c,13a, Ring, Ring9, c,13b, Ring, Ring7, c,14, c,15, c,15a, Ring, Ring8, c,15b, Ring, Ring4, c,16, c,17, c,17a, Ring, Ring5, C,18, c,18a, Ring, Ring1, Ring, Ring2
triphenylene|triphenylen root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a,

Ring, Ring3, c, 8b, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring4, c, 12b, Ring, Ring2, Ring, Ring1
trindene|trinden root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 3b, Ring, Ring3, c, 4, c, 5, c, 6, c, 6a, Ring, Ring4, c, 6b, Ring, Ring4, c, 7, c, 8, c, 9, c, 9a, Ring, Ring4, c, 9b, Ring, Ring2, Ring, Ring1
pyrene|pyren root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 8a, Ring, Ring4, c, 9, c, 10, c, 10a, Ring, Ring1, c, 10b, Ring, Ring2, c, 10c, Ring, Ring3, Ring, Ring4
chrysene|chrysen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 4b, Ring, Ring3, c, 5, c, 6, c, 6a, Ring, Ring4, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring4, c, 10b, Ring, Ring3, c, 11, c, 12, c, 12a, Ring, Ring2, Ring, Ring1
naphthacene|naphthacen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 5a, Ring, Ring3, c, 6, c, 6a, Ring, Ring4, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring4, c, 11, c, 11a, Ring, Ring3, c, 12, c, 12a, Ring, Ring2, Ring, Ring1
naphthaceno|naphthacen opfuser unknown
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 5a, Ring, Ring3, c, 6, c, 6a, Ring, Ring4, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring4, c, 11, c, 11a, Ring, Ring3, c, 12, c, 12a, Ring, Ring2, Ring, Ring1
pleiadene|pleiaden root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring3, c, 7, c, 7a, Ring, Ring4, c, 8, c, 9, c, 10, c, 11, c, 11a, Ring, Ring4, c, 12, c, 12a, Ring, Ring1, c, 12b, Ring, Ring3, Ring, Ring2
picene|picen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 6a, Ring, Ring3, c, 6b, Ring, Ring4, c, 7, c, 8, c, 8a, Ring, Ring5, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring5, c, 12b, Ring, Ring4, c, 13, c, 14, c, 14a, Ring, Ring3, c, 14b, Ring, Ring2, Ring, Ring1
perylene|perylen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring3, c, 6b, Ring, Ring4, c, 7, c, 8, c, 9, c, 9a, Ring, Ring5, c, 10, c, 11, c, 12, c, 12a, (, x, c, 12d, Ring, Ring5, Ring, Ring4,) , x, c, 12b, Ring, Ring1, c, 12c, Ring, Ring2, Ring, Ring3
peryllo opfuser unknown
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring3, c, 6b, Ring, Ring4, c, 7, c, 8, c, 9, c, 9a, Ring, Ring5, c, 10, c, 11, c, 12, c, 12a, (, x, c, 12d, Ring, Ring5, Ring, Ring4,) , x, c, 12b, Ring, Ring1, c, 12c, Ring, Ring2, Ring, Ring3
tetraphenylene|tetraphenylen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 4b, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 8b, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring4, c, 12b, Ring, Ring5, c, 13, c, 14, c, 15, c, 16, c, 16a, Ring, Ring5, c, 16b, Ring, Ring2, Ring, Ring1
rubicene|rubicen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 3b, Ring, Ring3, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring3, c, 7b, Ring, Ring4, c, 7c, Ring, Ring5, c, 8, c, 9, c, 10, c, 10a, Ring, Ring6, c, 10b, Ring, Ring7, c, 11, c, 12, c, 13, c, 14, c, 14a, Ring, Ring7, c, 14b, (, x, c, 14e, Ring, Ring6, Ring, Ring5,) , x, c, 14c, Ring, Ring1, c, 14d, Ring, Ring2, Ring, Ring4
coronene|coronen root root
c, 1, Ring, Ring1, c, 2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 4a, Ring, Ring3, c, 5, c, 6, c, 6a, Ring, Ring4, c, 7, c, 8, c, 8a, Ring, Ring5, c, 9, c, 10, c, 10a, Ring, Ring6, c, 11, c, 12, c, 12a, Ring, Ring1, c, 12b, Ring, Ring7, c, 12c, Ring, Ring2, c, 12d, Ring, Ring3, c, 12e, Ring, Ring4, c, 12f, Ring, Ring5, c, 12g, Ring, Ring6, Ring, Ring7
trinaphthylene|trinaphthylen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 5a, Ring, Ring3, c, 5b, Ring, Ring4, c, 6, c, 6a, Ring, Ring5, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring5, c, 11, c, 11a, Ring, Ring4, c, 11b, Ring, Ring6, c, 12, c, 12a, Ring, Ring7, c, 13, c, 14, c, 15, c, 16, c, 16a, Ring, Ring7, c, 17, c, 17a, Ring, Ring6, c, 17b, Ring, Ring3, c, 18, c, 18a, Ring, Ring2, Ring, Ring1

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pyranthrene|pyranthren root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,5a, Ring, Ring4, c
,6, c,7, c,7a, Ring, Ring5, c,8, c,8a, Ring, Ring6, c,9, c,10, c,11, c,12, c,12a, Ring, Ring6, c
,12b, Ring, Ring7, c,13, c,13a, Ring, Ring8, c,14, c,15, c,15a, (, x, c,16, c,16a, Ring, Ring2,
Ring, Ring1, ) , x, c,15b, Ring, Ring3, c,15c, Ring, Ring8, c,15d, Ring, Ring4, c,15e, Ring, Rin
g7, Ring, Ring5
ovalene|ovalen root root
c,1, Ring, Ring1, c,2, c,2a, Ring, Ring2, c,3, c,4, c,4a, Ring, Ring3, c,5, c,6, c,6a, Ring, Rin
g4, c,7, c,7a, Ring, Ring5, c,8, c,9, c,9a, Ring, Ring6, c,10, c,11, c,11a, Ring, Ring7, c,12, c
,13, c,13a, Ring, Ring8, c,14, c,14a, Ring, Ring1, c,14b, Ring, Ring9, c,14c, Ring, Ring2, c,1
4d, Ring, Ring3, c,14e, Ring, Ring4, c,14f, Ring, Ring0, c,14g, Ring, Ring5, c,14h, Ring, Ring
6, c,14i, Ring, Ring7, c,14j, Ring, Ring8, c,14k, Ring, Ring0, Ring, Ring9
biphenylene|biphenylen root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, c,4b, Ring, Ring3, c,5, c,6, c,7, c,8, c,8a,
Ring, Ring3, c,8b, Ring, Ring2, Ring, Ring1
thianthrene|thianthren root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, s,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
,9a, Ring, Ring3, s,10, c,10a, Ring, Ring2, Ring, Ring1
pyr root root
c,2|a|alpha, Ring, Ring1, c,3 b|beta, c,4|g|gamma, c,5, c,6, o,1, Ring, Ring1
pyrano opfuser unknown c,2, Ring, Ring1, c,3, c,4, c,5, c,6, o,1, Ring, Ring1
mdioxine|mdioxin root root c,2, Ring, Ring1, o,3, c,4, c,5, c,6, o,1, Ring, Ring1
pdioxine|pdioxin root root c,2, Ring, Ring1, c,3, o,4, c,5, c,6, o,1, Ring, Ring1
oxalene|oxalen root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, o,7, c,7a, Ring, Ring2, Ring, Ring
1
azalene|azalen root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, n,7, c,7a, Ring, Ring2, Ring, Ring
1
isobenzofuran root root
c,1, Ring, Ring1, o,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring2, Ring, Ring
1
benzofurazan root root
n,1, Ring, Ring1, o,2, n,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring2, Ring, Ring
1
benzofuroxan root root [n+],1, (, x, [O-
], x, ) , x, Ring, Ring1, o,2, n,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring2, Ring,
Ring1
piazhthiole root root
n,1, Ring, Ring1, s,2, n,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring2, Ring, Ring
1
catecholborane root root
o, x, Ring, Ring1, B, b, O, x, c,2, Ring, Ring2, c,3, c,4, c,5, c,6, c,1, Ring, Ring2, Ring, Ring1
chromene|chromen root root
c,2, Ring, Ring1, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring2, o,1, Ring,
Ring1
chromane|chroman root root
C,2, Ring, Ring1, C,3, C,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring2, O,1, Ring,
Ring1
chromone|chromon root root
c,2, Ring, Ring1, c,3, c,4, (=O) , x, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring2, o,
1, Ring, Ring1
esculetin root root
c,2, Ring, Ring1, (=O) , x, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, (O) , x, c,7, (O) , x, c,8, c,8a, R
ing, Ring2, o,1, Ring, Ring1

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umbelliferone root root
c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ri
ng2,o,1,Ring,Ring1
umbelliferyl root root
c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,4@7,c,8,c,8a,Ring,Ring2,
o,1,Ring,Ring1
isochromane|isochroman root root
C,1,Ring,Ring1,O,2,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
Ring2
flav root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,C,4|a-
l,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,)x,c,1',Ring,R
ing3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
flavone|flavon root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,)x,c,1'
,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
acacetin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',(OC),x,c,5',c,6',Ring,Ring3
alpinetin root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(OC),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
apigenin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
baicalein root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(O),x,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,R
ing,Ring1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
catechin root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
l,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,)x
,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
chrysin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
cirsiliol root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
,Ring,Ring1,)x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
diosmetin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
epicatechin root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
l,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,)x
,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
eupatorin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
,Ring,Ring1,)x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
galangin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
genkwanin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
hesperitin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
kaempferide|kaempferol root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,)x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3

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flavanone|flavanone root root C,2|a-t, (,x, Ring, Ring1, C,3|a-b, C,4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, O, 1, Ring, Ring1,) , x, c, 1'
, Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
anaphthoflavone|anaphthoflavon|alphanaphthoflavone|alphanaphthoflavon root root
O=C2C=C (C4=CC=CC=C4) OC1=C3C (C=CC=C3) =CC=C12, x
bnaphthoflavone|bnaphthoflavon|betanaphthoflavone|betanaphthoflavon root root
O=C2C=C (C3=CC=CC=C3) OC1=CC=C4C (C=CC=C4) =C12, x
xanthene|xanthen|xanthydr|xanth root root
c, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, o, 10, c, 10a, Ring, R
ing3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
xanthone|xanthon root root
c, 9, Ring, Ring1, (, x, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, o, 10, c, 10a, Ri
ng, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1,) , x, =O, x
xanthylum root root
c, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [o+], 10, c, 10a, Rin
g, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
xanthuren root root
C, x, c, 2, Ring, Ring1, c, 3, c, 4, (O), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, (O), x, c, 8a, Ring
, Ring2, n, 1, Ring, Ring1
thioxanthene|thioxanthen root root
c, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, s, 10, c, 10a, Ring, R
ing3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
selenoxanthene|selenoxanthen root root
c, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [se], 10, c, 10a, Rin
g, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
acridars root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [as], 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c,
9, c, 9a, Ring, Ring3, c, 10, c, 10a, Ring, Ring2, Ring, Ring1
arsanthrene|arsanthren root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [as], 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c,
9, c, 9a, Ring, Ring3, [as], 10, c, 10a, Ring, Ring2, Ring, Ring1
phosphanthrene|phosphanthren root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, p, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, p, 10, c, 10a, Ring, Ring2, Ring, Ring1
selenanthrene|selenanthren root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [se], 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c,
9, c, 9a, Ring, Ring3, [se], 10, c, 10a, Ring, Ring2, Ring, Ring1
phenomercurin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [Hg], 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c,
9, c, 9a, Ring, Ring3, [Hg], 10, c, 10a, Ring, Ring2, Ring, Ring1
phenoxathiin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, o, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, s, 10, c, 10a, Ring, Ring2, Ring, Ring1
phenoxastannin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, [Sn], 10, c, 10a, Ring, Ring2, Ring, Ring1
phenoxasilin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, [Si], 10, c, 10a, Ring, Ring2, Ring, Ring1
phenoxagermanin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, [Ge], 10, c, 10a, Ring, Ring2, Ring, Ring1
phenothiastannin root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, S, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c
, 9a, Ring, Ring3, [Sn], 10, c, 10a, Ring, Ring2, Ring, Ring1

phenothiasilin root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, S,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Si], 10, c,10a, Ring, Ring2, Ring, Ring1
phenothiagermanin root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, S,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Ge], 10, c,10a, Ring, Ring2, Ring, Ring1
phenaz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, n,10, c,10a, Ring, Ring2, Ring, Ring1
phenazasilin|phenazasilin root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, N,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Si], 10, c,10a, Ring, Ring2, Ring, Ring1
phenarsaz|phenoarsaz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [as], 10, c,10a, Ring, Ring2, Ring, Ring1
phenothiaz|thiodiphenylamine root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, s,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, n,10, c,10a, Ring, Ring2, Ring, Ring1
phenomercaz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, N,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Hg], 10, c,10a, Ring, Ring2, Ring, Ring1
phenophosphaz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, p,10, c,10a, Ring, Ring2, Ring, Ring1
phenotelluraz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, [Te], 5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, N,10, c,10a, Ring, Ring2, Ring, Ring1
phenoselenaz root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, [Se], 5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, N,10, c,10a, Ring, Ring2, Ring, Ring1
phenothiars root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, s,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [as], 10, c,10a, Ring, Ring2, Ring, Ring1
phenoxantimon root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Sb], 10, c,10a, Ring, Ring2, Ring, Ring1
phenoxars root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [as], 10, c,10a, Ring, Ring2, Ring, Ring1
phenoxaphos root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, P,10, c,10a, Ring, Ring2, Ring, Ring1
phenoxatellur root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Te], 10, c,10a, Ring, Ring2, Ring, Ring1
phenoxaselen root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, [Se], 10, c,10a, Ring, Ring2, Ring, Ring1
dibenzodioxin root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, o,10, c,10a, Ring, Ring2, Ring, Ring1
phenoxaz|phenazox root root
c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,9, c,9a, Ring, Ring3, n,10, c,10a, Ring, Ring2, Ring, Ring1
indene|inden root root
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2

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indeno opfuser unknown
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
indole|indol root root
n,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
thianaphthene|thianaphthen|thionaphthene|thionaphthen root root
s,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
thianaphtheno|thianaphthen opfuser unknown
s,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
isothianaphthene|isothianaphthen root root
c,1, Ring, Ring1, s,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
isothianaphtheno|isothianaphthen opfuser unknown
c,1, Ring, Ring1, s,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
skatole|skatol root root
n,1, Ring, Ring1, c,2, c,3, (C), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Rin
g, Ring2
gramine root root
n,1, Ring, Ring1, c,2, c,3, (CN(C)C), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring
1, Ring, Ring2
indolo opfuser unknown
n,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isoindole|isoindol root root
c,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isoindolo opfuser unknown
c,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
arsindole|arsindol root root
[as],1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
arsindolo opfuser unknown
[as],1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
isoarsindole|isoarsindol root root
c,1, Ring, Ring1, [as],2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
isoarsindolo|isoarsindol opfuser unknown
c,1, Ring, Ring1, [as],2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
phosphindole|arsindol root root
p,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
phosphindolo|arsindol opfuser unknown
p,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isophosphindole|isoarsindol root root
c,1, Ring, Ring1, p,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isophosphindolo|isoarsindol opfuser unknown
c,1, Ring, Ring1, p,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2

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indazole|indazol root root
n,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indazolo|indazol opfuser unknown
n,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indolizine|indolizin|pyrrocol root root
c,1, Ring, Ring1, c,2, c,3, n,4, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
indolizino opfuser unknown
c,1, Ring, Ring1, c,2, c,3, n,4, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
oxindole|oxindol root root
N,1, Ring, Ring1, C,2, (=, x, O, x,) , x, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indoline|indolin root root
N,1, Ring, Ring1, C,2, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
isat root root
N,1, Ring, Ring1, C,2|alpha, (=O) , x, C,3|beta, (=O) , x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
isoindoline|isoindolin root root
C,1, Ring, Ring1, N,2, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indane|indan|hydrindene|hydrind root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
hydrindantin root root O=C(c2c1cccc2)C(C1=O)(O)C(C3=O)(O)C(c4c3cccc4)=O, x
alloxantin root root OC1(C2(C(NC(NC2=O)=O)=O)O)C(NC(NC1=O)=O)=O, x
ninhydrin root root
C,1, (=O) , x, Ring, Ring1, C,2, (=O) , x, C,3, (=O) , x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
tetral root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, C,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
decal root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, C,4, C,10, Ring, Ring2, C,5, C,6, C,7, C,8, C,9, Ring, Ring1, Ring, Ring2
hexalin root root C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, Ring, Ring1
quinol|chinol|quinolin|chinolin|leucol root root
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
quinolin|chinolin opfuser unknown
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
carbostyryl|carbostyryl root root
n,1, Ring, Ring1, c,2|b|beta, (O) , x, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
isocarbostyryl|isocarbostyryl root root
c,1, (O) , x, Ring, Ring1, n,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
lepid root root
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, (C) , x, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
cinchonin loveracid root
c,4, Ring, Ring1, c,3, c,2, n,1, c,8a, Ring, Ring2, c,8, c,7, c,6, c,5, c,4a, Ring, Ring1, Ring, Ring2

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quino|chino opfuser unknown
n,1, Ring, Ring1, c, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
quinald|chinald root root
C, a |alpha, Ring, Ring3, ., x, n, 1, Ring, Ring1, c, 2 |b| beta, Ring, Ring3, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
xanthur root root
C, a |alpha, Ring, Ring3, ., x, n, 1, Ring, Ring1, c, 2 |b| beta, Ring, Ring3, c, 3, c, 4, (O), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, (O), x, c, 8a, Ring, Ring1, Ring, Ring2
quinoliz|chinoliz root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, n, 5, Ring, Ring2, c, 6, c, 7, c, 8, c, 9, c, 8a, Ring, Ring2, Ring, Ring1
quinazol|chinazol root root
n, 1, Ring, Ring1, c, 2 |b| beta, n, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
quinazol|chinazol|quinazolino opfuser unknown
n, 1, Ring, Ring1, c, 2 |b| beta, n, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
isoquinol|isochinol root root
c, 1 |a| alpha, Ring, Ring1, n, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
isoquino|isochino opfuser unknown
c, 1 |a| alpha, Ring, Ring1, n, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
cinnol root root
n, 1, Ring, Ring1, n, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
quinoxal|chinoxal|phenpiaz root root
n, 1, Ring, Ring1, c, 2 |b| beta, c, 3, n, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
arsinol root root
[as], 1, Ring, Ring1, c, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
isoarsinol root root
c, 1 |a| alpha, Ring, Ring1, [as], 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
phosphinol root root
p, 1, Ring, Ring1, c, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
isophosphiol root root
c, 1 |a| alpha, Ring, Ring1, p, 2 |b| beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
pterid root root
n, 1, Ring, Ring1, c, 2 |b| beta, n, 3, c, 4, c, 4a, Ring, Ring2, n, 5, c, 6, c, 7, n, 8, c, 8a, Ring, Ring1, Ring, Ring2
phthalazine|phthalazin root root
c, 1 |a| alpha, Ring, Ring1, n, 2 |b| beta, n, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
phthalhydrazide root root
C, x, Ring, Ring1, (=O), x, N, x, N, x, C, x, (=O), x, c, 2, Ring, Ring2, c, 3, c, 4, c, 5, c, 6, c, 1, Ring, Ring1, Ring, Ring2
fluorene|fluoren root root
c, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
diphenyleneiodonium root root
[I+], 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1

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betacarboline root root
c,1, Ring, Ring1, n, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 4b, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, n, 9 | prefhydro, c, 9a, Ring, Ring2, Ring, Ring1
carbazole | carbazol root root
n, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
carbazolo | carbazol ofuser unknown
n, 9, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
norharman root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, n, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmaline | harman root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, (C), x, n, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmine | banisterine root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, (C), x, n, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmol root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, (C), x, n, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmalol root root
N, 9, Ring, Ring1, C, 9a, Ring, Ring2, C, 1, (C), x, =, x, N, 2, C, 3, C, 4, C, 4a, (, x, =, x, Ring, Ring2,), x, c, 4b, Ring, Ring3, c, 5, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmaline root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, (C), x, n, 2, C, 3, C, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
harmalane | harmalan root root
n, 9 | prefhydro, Ring, Ring1, c, 9a, Ring, Ring2, c, 1, (C), x, n, 2, C, 3, C, 4, c, 4a, Ring, Ring2, c, 5a, Ring, Ring3, c, 5, c, 6, (OC), x, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
phenanthrid root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, n, 5, c, 6, c, 6a, Ring, Ring3, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring3, c, 10b, Ring, Ring2, Ring, Ring1
arsanthrid root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, [as], 5, c, 6, c, 6a, Ring, Ring3, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring3, c, 10b, Ring, Ring2, Ring, Ring1
benzidine | benzin root root
N, n, c, 4, Ring, Ring1, c, 3, c, 2, c, 1, (, x, c, 6, c, 5, Ring, Ring1,), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', (, x, N, n',), x, c, 5', c, 6', Ring, Ring2
benzidinium root root
[N+], n, c, 4, Ring, Ring1, c, 3, c, 2, c, 1, (, x, c, 6, c, 5, Ring, Ring1,), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', (, x, [N+], n',), x, c, 5', c, 6', Ring, Ring2
benzidino root root
N, 4@n, c, 4, Ring, Ring1, c, 3, c, 2, c, 1, (, x, c, 6, c, 5, Ring, Ring1,), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', (, x, N, n',), x, c, 5', c, 6', Ring, Ring2
pyrid root root
c, 2 | o | ortho | a | alpha, Ring, Ring1, c, 3 | m | meta | b | beta, c, 4 | p | para | g | gamma, c, 5, c, 6, n, 1 | n, Ring, Ring1
pyrido | pyrid ofuser unknown
c, 2 | o | ortho | a | alpha, Ring, Ring1, c, 3 | m | meta | b | beta, c, 4 | p | para | g | gamma, c, 5, c, 6, n, 1 | n, Ring, Ring1
pyridox root root
C, 4, c, x, Ring, Ring1, c, x, (, x, C, 5, O, x,), x, c, 6, n, 1, c, 2, (C), x, c, 3, (O), x, Ring, Ring1
pyridoxamine | pyridoxamin root root
N, x, C, 4, c, x, Ring, Ring1, c, x, (, x, C, 5, O, x,), x, c, 6, n, 1, c, 2, (C), x, c, 3, (O), x, Ring, Ring1

pyraz root root
c,2|o|ortho, Ring, Ring1, c,3|m|meta, Ring, Ring2, ., x, n,1|n, Ring, Ring3, Ring, Ring1, ., x
, n,4|p|para|n', Ring, Ring2, c,5, c,6, Ring, Ring3
pyrazino ofuser unknown
c,2|o|ortho, Ring, Ring1, c,3|m|meta, n,4|p|para, c,5, c,6, n,1|n, Ring, Ring1
pyrimid root root
c,2|o|ortho, Ring, Ring1, n,3 m|meta, c,4|p|para, c,5, c,6, n,1|n, Ring, Ring1
pyrimido|pyrimid ofuser unknown
c,2|o|ortho, Ring, Ring1, n,3|m|meta, c,4|p|para, c,5, c,6, n,1|n, Ring, Ring1
pyridaz root root c,3, Ring, Ring1, c,4, c,5, c,6, n,1|n, n,2|n', Ring, Ring1
pyridazo|pyridazino ofuser unknown
c,3, Ring, Ring1, c,4, c,5, c,6, n,1|n, n,2|n', Ring, Ring1
striazone|striazin|symtriazone|symtriazin root root
c,2, Ring, Ring1, n,3, c,4, n,5, c,6, n,1, Ring, Ring1
astriazone|astriazin|asymtriazone|asymtriazin root root
n,2, Ring, Ring1, c,3, n,4, c,5, c,6, n,1, Ring, Ring1
strixane|strixan|symstrixane|symstrixan root root
C,2, Ring, Ring1, O,3, C,4, O,5, C,6, O,1, Ring, Ring1
astrixane|astrixan|asymstrixane|asymstrixan root root
O,2, Ring, Ring1, C,3, O,4, C,5, C,6, O,1, Ring, Ring1
strithiane|strithian|symtrithiane|symtrithian root root
C,2, Ring, Ring1, S,3, C,4, S,5, C,6, S,1, Ring, Ring1
astrithiane|astrithian|asymtrithiane|asymtrithian root root
S,2, Ring, Ring1, C,3, S,4, C,5, C,6, S,1, Ring, Ring1
striazone|symtriazone ofuser unknown
c,2, Ring, Ring1, n,3, c,4, n,5, c,6, n,1, Ring, Ring1
astriazone|asymtriazone ofuser unknown
n,2, Ring, Ring1, c,3, n,4, c,5, c,6, n,1, Ring, Ring1
strixano|symstrixano ofuser unknown
C,2, Ring, Ring1, O,3, C,4, O,5, C,6, O,1, Ring, Ring1
astrixano|asymstrixano ofuser unknown
O,2, Ring, Ring1, C,3, O,4, C,5, C,6, O,1, Ring, Ring1
strithiano|symtrithiano ofuser unknown
C,2, Ring, Ring1, S,3, C,4, S,5, C,6, S,1, Ring, Ring1
astrithiano|asymtrithiano ofuser unknown
S,2, Ring, Ring1, C,3, S,4, C,5, C,6, S,1, Ring, Ring1
borazine|borazin root root N,1, Ring, Ring1, [B],2, N,3, [B],6, Ring, Ring1
phosphazine|borazin root root n,2, Ring, Ring1, p,3, n,4, p,5, n,6, p,1, Ring, Ring1
pyrrole|pyrrol root root r,1, Ring, Ring1, c,2, c,3, c,4, c,5, Ring, Ring1
pyrrolo|pyrrol ofuser unknown n,1, Ring, Ring1, c,2, c,3, c,4, c,5, Ring, Ring1
pyrrolid root root N,1, Ring, Ring1, C,2|a|alpha, C,3|b|beta, C,4, C,5, Ring, Ring1
pyrrolidino root root N,4@1, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
imidazole|imidazol|glyoxaline|glyoxalin root root
c,2, Ring, Ring1, n,3, c,4, =, x, c,5, n,1|prefhydro, Ring, Ring1
imidazolo|imidazol|imidazo|imidaz ofuser unknown
c,2, Ring, Ring1, n,3, c,4, =, x, c,5, n,1, Ring, Ring1
imidazolid root root C,2, Ring, Ring1, N,3, C,4, C,5, N,1, Ring, Ring1
pyrazole|pyrazol root root n,1, Ring, Ring1, n,2, c,3, c,4, c,5, Ring, Ring1
pyrazolo|pyrazol ofuser unknown n,1, Ring, Ring1, n,2, c,3, c,4, c,5, Ring, Ring1
tetrazolium root root n,1, Ring, Ring1, [n+],2, n,3, n,4, c,5, Ring, Ring1
pyrazabole|pyrazabol root root
c,1, Ring, Ring1, c,2, c,3, n,3a, n,8a, (, x, [B],8,) x, Ring, Ring1, ., x, [B],4, n,4a, Ring, Ri
ng2, c,5, c,6, c,7, n,7a, Ring, Ring2
isooxazole|isooxazol|isoxazole|isoxazol|isoazole|isoazol root root
o,1, Ring, Ring1, n,2, c,3, c,4, c,5, Ring, Ring1
isooxazolo|isooxazol|isoxazolo|isoxazol ofuser unknown
o,1, Ring, Ring1, n,2, c,3, c,4, c,5, Ring, Ring1

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isooxazolid|isooxazolid|isoxazolid|isoxazolid|isoazolid|isoazolid root root
O,1, Ring, Ring1, N, 2, C, 3, C, 4, C, 5, Ring, Ring1
urazole|urazol root root N,1, Ring, Ring1, N, 2, C, 3, (=O), x, N, 4, C, 5, (=O), x, Ring, Ring1
pyrazolid root root N,1, Ring, Ring1, N, 2, C, 3, C, 4, C, 5, Ring, Ring1
furan|fur root root o,1, Ring, Ring1, c, 2|a|alpha, c, 3|b|beta, c, 4, c, 5, Ring, Ring1
furo opfuser unknown o,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
furfur root root C, a|alpha, c, 2, Ring, Ring1, c, 3, c, 4, c, 5, o, 1, Ring, Ring1
then root root C, 2, c, x, Ring, Ring1, c, 3, c, 4, c, 5, s, 1, Ring, Ring1
furazan root root c, 3, Ring, Ring1, c, 4, n, 5, o, 1, n, 2, Ring, Ring1
isothiazole|isothiazol root root s, 1, Ring, Ring1, n, 2, c, 3, c, 4, c, 5, Ring, Ring1
isothiazolo|isothiazol opfuser unknown s, 1, Ring, Ring1, n, 2, c, 3, c, 4, c, 5, Ring, Ring1
isosulfonazole|isosulfonazol root root
c, 4, Ring, Ring1, c, 5, s, 1, (=, x, O, x,) (=, x, O, x,) x, n, 2, c, 3, Ring, Ring1
isoselenazole|isoselenazol root root
[se], 1, Ring, Ring1, n, 2, c, 3, c, 4, c, 5, Ring, Ring1
isoselenazolo|isoselenazol opfuser unknown
[se], 1, Ring, Ring1, n, 2, c, 3, c, 4, c, 5, Ring, Ring1
benzisosulfonazole|benzisosulfonazol root root
s, 1, (=, x, O, x,) (=, x, O, x,) x, Ring, Ring1, n, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c,
7a, Ring, Ring2, Ring, Ring1
benzsulfonazole|benzsulfonazol root root
s, 1, (=, x, O, x,) (=, x, O, x,) x, Ring, Ring1, c, 2, n, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c,
7a, Ring, Ring2, Ring, Ring1
sulfonazole|sulfonazol root root
s, 1, (=, x, O, x,) (=, x, O, x,) x, Ring, Ring1, c, 2, n, 3, c, 4, c, 5, Ring, Ring1
thiophene|thien root root
c, 2|a|alpha, Ring, Ring1, c, 3|b|beta, c, 4, c, 5, s, 1, Ring, Ring1
thieno|thien opfuser unknown c, 2, Ring, Ring1, c, 3, c, 4, c, 5, s, 1, Ring, Ring1
selenophene|selenophen root root [se], 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
selenopheno|selenophen opfuser unknown
[se], 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
tellurophene|tellurophen root root [Te], 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
telluropheno|tellurophen opfuser unknown
[Te], 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
piperid root root N, 1|n, Ring, Ring1, C, 2, C, 3, C, 4, C, 5, C, 6, Ring, Ring1
piperidino root root N, 4@1|n, Ring, Ring1, C, 2, C, 3, C, 4, C, 5, C, 6, Ring, Ring1
homopiperid root root N, 1|n, Ring, Ring1, C, 2, C, 3, C, 4, C, 5, C, 6, C, 7, Ring, Ring1
nipecot root root C, a|alpha, C, 3, Ring, Ring1, C, 4, C, 5, C, 6, N, 1|n, C, 2, Ring, Ring1
isonipecot root root C, a|alpha, C, 4, Ring, Ring1, C, 5, C, 6, N, 1|n, C, 2, C, 3, Ring, Ring1
purine|purin root root
n, 7|prefhydro, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, c, 2, n, 1, c, 6, c, 5, Ring, Ring1, R
ing, Ring2
adenine|adenin root root
n, 1, Ring, Ring1, c, 2, n, 3, c, 4, (, x, c, 5, Ring, Ring2, c, 6, (, x, N, n|n6, ), x, Ring, Ring1, ), x,
n, 9, c, 8, n, 7|prefhydro, Ring, Ring2
piperaz root root N, 1|n, Ring, Ring1, C, 2, C, 3, N, 4|n', C, 5, C, 6, Ring, Ring1
piperazino root root N, 4@1|n, Ring, Ring1, C, 2, C, 3, N, 4, C, 5, C, 6, Ring, Ring1
homopiperaz root root N, 1|n, Ring, Ring1, C, 2, C, 3, N, 4, C, 5, C, 6, C, 7, Ring, Ring1
homopiperazino root root N, 4@1|n, Ring, Ring1, C, 2, C, 3, N, 4, C, 5, C, 6, C, 7, Ring, Ring1
pyrroliz root root
n, 4, Ring, Ring1, Ring, Ring2, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, c, 1, c, 2, c, 3, Ring, Ring2
pentalene|pentalen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring1, Ring, Ring2
pentaleno|pentalen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 6a, Ring, Ring1, Ring, Ring2

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heptalene|heptalen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 5a, Ring, Ring2, c, 6, c, 7, c, 8, c, 9, c, 10, c, 10a, Ring, Ring1, Ring, Ring2
asindacene|asindacen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 8b, Ring, Ring2, Ring, Ring1
sindacene|sindacen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 4a, Ring, Ring3, c, 5, c, 6, c, 7, c, 7a, Ring, Ring3, c, 8, c, 8a, Ring, Ring2, Ring, Ring1
octalene|octalen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 6a, Ring, Ring2, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring1, Ring, Ring2
mevalon root root C,1,C,2,C,3,(,x,C,4,C,5,O,x),(,x,O,x),x,C,x
lact|lactyl root root C,1,C,2|alpha|a,(,x,O,x),x,C,3|b|beta
24d root root
O,1@x,C,x,(=,x,O,x),x,C,a|alpha,O,x,c,1, Ring, Ring1, c, 2, (,x,C1,x),x,c,3,c,4,(,x,C1,x),x,c,5,c,6, Ring, Ring1
245t root root
O,1@x,C,x,(=,x,O,x),x,C,a|alpha,O,x,c,1, Ring, Ring1, c, 2, (,x,C1,x),x,c,3,c,4,(,x,C1,x),x,c,5,(,x,C1,x),x,c,6, Ring, Ring1
dnp|24dnp root root c,4@1, Ring, Ring1, c, x, ([N+](=O)[O-]),x,c,3|m|meta,c,x,([N+](=O)[O-]),x,c,5,c,6, Ring, Ring1
morphol root root C,2, Ring, Ring1, C,3,N,4,C,5,C,6,O,1, Ring, Ring1
morpholino root root O,1, Ring, Ring1, C,2,C,3,N,4@4,C,5,C,6, Ring, Ring1
semicarbazide|semicarbazid root root N,1,N,2,C,x,(=,x,O,3),x,N,4
semicarbazido root root N,4@1,N,2,C,x,(=,x,O,3),x,N,4
isosemicarbazide|isosemicarbazid root root N,1,N,2,C,x,(,x,O,3),=,x,N,4
isosemicarbazido root root N,4@1,N,2,C,x,(,x,O,3),=,x,N,4
semicarbazono root root N,3@1,N,2,C,x,(=,x,O,3),x,N,4
carbaz root root C,1,N,2,N,3
acetone|aceton root alkane C,1|a|alpha,C,x,(=O),x,C,3|w|omega
acetylacetone root root C,1,C,2,(=,x,O,x),x,C,3,C,4,(=,x,O,x),x,C,5
isobutyronone|isobutyron root root CC(C)C(=O)C(C)C,x
isovaleronone|isovaleron root root CC(C)CC(=O)CC(C)C,x
enanthonone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,(=O),x,C,8,C,9,C,10,C,11,C,12,C,13|w|omega
pelargone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(=O),x,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
laurone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,x,(=O),x,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23|w|omega
myristone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,x,(=O),x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27|w|omega
palmitone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,x,(=O),x,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31|w|omega
stearone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,x,(=O),x,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31,C,32,C,33,C,34,C,35|w|omega
silatrane|silatran root root
[Si],1, Ring, Ring1, Ring, Ring2, O,2,C,3,C,4,N,5,(,x,C,6,C,7,O,8, Ring, Ring1),x,C,11,C,10,O,9, Ring, Ring2

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glycoluril root root
N,n|1, Ring, Ring1, C, 2, (=, x, O, x, ), x, N, n' |3, C, 3a, Ring, Ring2, N, n' ' |4, C, 5, (=, x, O, x, ),
x, N, n' ' ' |6, C, 6a, Ring, Ring1, Ring, Ring2
acetylene|acetylen root root C, 1, #, x, C, 2
diacetylene root root C, 1, #, x, C, 2, C, 3, #, x, C, 4
allophan root trivial C, 1, (=, x, O, x, ), x, N, 2, C, 3, (=, x, O, x, ), x, N, 4
biguanide|biguanid root root N, 1, C, x, (=, x, N, 2, ), x, N, 3, C, x, (=, x, N, 4, ), x, N, 5
biuret root root N, 1, C, 2, (=, x, O, x, ), x, N, 3, C, 4, (=, x, O, x, ), x, N, 5
carbazone|carbazon root root N, 1, N, 2, C, 3, (=, x, O, x, ), x, N, 4, =, x, N, 5
carbazono root root N, 4@1, N, 2, C, 3, (=, x, O, x, ), x, N, 4, =, x, N, 5
carbodiazone|carbodiazon root root N, 1, =, x, N, 2, C, 3, (=, x, O, x, ), x, N, 4, =, x, N, 5
carbodiazone root root N, 4@1, =, x, N, 2, C, 3, (=, x, O, x, ), x, N, 4, =, x, N, 5
carbodiimide|carbodiimid root root N, n|1, =, x, C, x, =, x, N, n' |3
sulfurdiimide|sulfurdiimid root root N, n|1, =, x, S, x, =, x, N, n' |3
carbonohydrazide|carbonohydrazid|carbohydrazide|carbohydrazid|carbazide|carbazid
root root N, 1, N, 2, C, 3, (=, x, O, x, ), x, N, 4, N, 5
carbonohydrazido|carbohydrazido|carbazido root root
N, 4@1, N, 2, C, x, (=, x, O, x, ), x, N, 4, N, 5
isocarbonohydrazide|isocarbonohydrazid root root
N, 1, N, 2, C, x, (=, x, O, x, ), x, N, 4, N, 5
isocarbonohydrazido root root N, 4@1, N, 2, C, x, (=, x, O, x, ), x, N, 4, N, 5
formazan root root N, 1, N, 2, =, x, C, 3, N, 4, =, x, N, 5
guanidine|guanidin root root N, 1|n, C, x, (=, x, N, 3|n' ), x, =, x, N, 2|n'
guanidino|guanido root root N, 4@1, C, x, (=, x, N, 2, ), x, N, 3
hydanto|hydant root root C, 1, C, 2, N, 3, C, 4, (=, x, O, x, ), x, N, 5
hydantoin root root
N, 1, Ring, Ring1, C, 2, (=, x, O, x, ), x, N, 3, C, 4, (=, x, O, x, ), x, C, 5, Ring, Ring1
rhodanine|rhodanin root root
S, 1, Ring, Ring1, C, 2, (=, x, S, x, ), x, N, 3, C, 4, (=, x, O, x, ), x, C, 5, Ring, Ring1
isourea|pseudourea root root N, 1|n, =, x, C, x, (=, x, O, 2, ), x, N, 3|n'
1isoureido root root N, 4@1|n, =, x, C, x, (=, x, O, o, ), x, N, 3|n'
3isoureido root root N, 1|n, =, x, C, x, (=, x, O, o, ), x, N, 4@3|n'
isothiurea root root N, 1|n, =, x, C, x, (=, x, S, s, ), x, N, 3|n'
isothiuronium root root N, 1|n, =, x, C, x, (=, x, [S+], s, ), x, N, 3|n'
1isothioureido root root N, 4@1|n, =, x, C, x, (=, x, S, s, ), x, N, 3|n'
3isothioureido root root N, 1|n, =, x, C, x, (=, x, S, s, ), x, N, 4@3|n'
isoselenourea root root N, 1|n, =, x, C, x, (=, x, [Se], se, ), x, N, 3|n'
isoselenouronium root root N, 1|n, =, x, C, x, (=, x, [Se+], se, ), x, N, 3|n'
1isoselenoureido root root N, 4@1|n, =, x, C, x, (=, x, [Se], se, ), x, N, 3|n'
3isoselenoureido root root N, 1|n, =, x, C, x, (=, x, [Se], se, ), x, N, 4@3|n'
isotellurourea root root N, 1|n, =, x, C, x, (=, x, [Te], te, ), x, N, 3|n'
isotellurouronium root root N, 1|n, =, x, C, x, (=, x, [Te+], te, ), x, N, 3|n'
1isotelluroureido root root N, 4@1|n, =, x, C, x, (=, x, [Te], te, ), x, N, 3|n'
3isotelluroureido root root N, 1|n, =, x, C, x, (=, x, [Te], te, ), x, N, 4@3|n'
glycer pseudosugar unknown x, x
glycer root root C, 1, C, 2, (=, x, O, a|alpha, ), x, C, 3, O, b|beta,
pentaerythritol root root O, x, C, x, C, x, (=, x, C, x, O, x, ), x, (=, x, C, x, O, x, ), x, C, x, O, x
pentaerythrityl root root C, 4@x, C, x, (=, x, C, 4@x, ), x, (=, x, C, 4@x, ), x, C, 4@x
alphapinene root root
C, 1, Ring, Ring1, Ring, Ring2, C, 2, (=, x, C, 10, ), x, C, 3, C, 4, C, 5, (=, x, C, 6, Ring, Ring1, ), x, C
, 7, (=, x, C, 8, ), x, (=, x, C, 9, ), x, Ring, Ring2
betapinene root root
C, 1, Ring, Ring1, Ring, Ring2, C, 2, (=, x, C, 10, ), x, C, 3, C, 4, C, 5, (=, x, C, 6, Ring, Ring1, ), x, C
, 7, (=, x, C, 8, ), x, (=, x, C, 9, ), x, Ring, Ring2
carve|carv|carvene root root
C, 2, Ring, Ring1, C, 3, C, 4, (=, x, C, 8, (=, x, C, 9, ), x, C, 10, ), x, C, 5, c, 6, c, 1, (=, x, C, 7, ), x, Rin
g, Ring1

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isocoumarin|isocoumarin root root
C,1, Ring, Ring1, (=, x, O, x, ), x, o, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
coumaran root root
O,1, Ring, Ring1, C, 2, C, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
coumarone|coumaron root root
o,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
ayapin root root
o,1, Ring, Ring1, c, 2, (=, x, O, x, ), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, (, x, COC, x, Ring, Ring3, ), x, c, 7, Ring, Ring3, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
benzhydr root root
C, a|alpha, (, x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
benzoguanamine|benzoguanamin root root
c, 1, (, x, Ring, Ring1, n, 2, c, 3, (, x, N, x, ), x, n, 4, c, 5, (, x, N, x, ), x, n, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
trit root root
C, a|alpha, Ring, Ring1, Ring, Ring2, Ring, Ring3, ., x, c, 4, Ring, Ring4, Ring, Ring5, ., x, c, 4', Ring, Ring6, Ring, Ring7, ., x, c, 4'', Ring, Ring8, Ring, Ring9, ., x, c, 3, Ring, Ring4, c, 2, c, 1, Ring, Ring1, c, 6, c, 5, Ring, Ring5, ., x, c, 3', Ring, Ring6, c, 2', c, 1', Ring, Ring2, c, 6', c, 5', Ring, Ring7, ., x, c, 3'', Ring, Ring8, c, 2'', c, 1'', Ring, Ring3, c, 6'', c, 5'', Ring, Ring9
ureth root root N, n, C, x, (=, x, O, x, ), x, O, x, C, x, C, x
chalcone|chalcon root root
C, a|alpha, (, x, C, x, (=, x, O, x, ), x, c, 1', Ring, Ring1, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring1, ), x, =, x, C, b|beta, c, 1, Ring, Ring2, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring2
deoxybenzoin root root
C, a|alpha, (, x, C, x, (=O), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, =, x, C, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
thiurammonosulfide|thiurammonosulfid root root
N, n, C, x, (=, x, S, x, ), x, S, x, C, x, (=, x, S, x, ), x, N, n'
thiuramdisulfide|thiuramdisulfid root root
N, n, C, x, (=, x, S, x, ), x, SS, x, C, x, (=, x, S, x, ), x, N, n'
thiuramtrisulfide|thiuramtrisulfid root root
N, n, C, x, (=, x, S, x, ), x, SSS, x, C, x, (=, x, S, x, ), x, N, n'
thiuramtetrasulfide|thiuramtetrasulfid root root
N, n, C, x, (=, x, S, x, ), x, SSSS, x, C, x, (=, x, S, x, ), x, N, n'
mercuran root root S=C(SSC(N(C)C)=S)N(C)C, x
diacetamide|diacetamid root root
N, n, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, C, x, (, x, =, x, O, x, ), x, C, x
triacetamide|triacetamid root root
N, x, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, C, x, (, x, =, x, O, x, ), x, C, x
dibenzamide|dibenzamid root root
N, n, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring1, ccccc, x, Ring, Ring1, ), x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring2, ccccc, x, Ring, Ring2
tribenzamide|tribenzamid root root
N, x, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring1, ccccc, x, Ring, Ring1, ), x, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring2, ccccc, x, Ring, Ring2, ), x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring3, =, x, ccccc, x, Ring, Ring3
fulvene|fulven root root
C, 6, =, x, C, 5, Ring, Ring1, C, 1, =, x, C, 2, C, 3, =, x, C, 4, Ring, Ring1
stilbene|stilben root root
C, b|beta|a'|alpha', (=, x, C, a|alpha, c, 1, Ring, Ring1, c, 2|o|ortho, c, 3|m|meta, c, 4|p|para,
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ra,c,5,c,6, Ring, Ring1, ) , x, c, 1', Ring, Ring2, c, 2' | o' | ortho', c, 3' | m' | meta', c, 4' | p' | p
ara', c, 5', c, 6', Ring, Ring2
stilbestrol|stilboestrol root root
C, b|beta, (=, x, C, a|alpha, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, (O), x, c, 5, c, 6, Ring, Ring1, ) , x,
c, 1', Ring, Ring2, c, 2', c, 3', c, 4', (O), x, c, 5', c, 6', Ring, Ring2
hexestrol root root
C, b|beta, (CC) (, x, C, a|alpha, (CC) , x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, (O), x, c, 5, c, 6, Ring,
Ring1, ) , x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', (O), x, c, 5', c, 6', Ring, Ring2
benzil root root
C(=O), x, (, x, C(=O), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1, ) , x, c, 1', Ring,
Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
antipyr|antipyrene|phenazone root root
C, 4, Ring, Ring1, c, 5, (=O), x, N, 1, (, x, N, 2, (, x, C, x, ) , x, C, 3, (, x, C, x, ) , x, =, x, Ring, Ring1
, ) , x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
glycid root root C, 1, C, 2 | b|beta, Ring, Ring1, C, 3, O, x, Ring, Ring1
ketene|keten root root C=C=O, 1
diketene|diketen root root C=C1CC(=O)O1, x
adamant root root
C, 1, Ring, Ring1, Ring, Ring2, C, 2, C, 3, Ring, Ring3, C, 4, C, 5, (, x, C, 6, C, 7, (, x, C, 8, Ring, Ri
ng1, ) , x, C, 10, Ring, Ring3, ) , x, C, 9, Ring, Ring2
noradamant root root
C, 1, Ring, Ring1, Ring, Ring2, C, 2, C, 3, Ring, Ring3, C, 4, C, 5, (, x, C, 6, C, 7, (, x, C, 8, Ring, Ri
ng1, ) , x, Ring, Ring3, ) , x, C, 9, Ring, Ring2
hexamethylenetetramine|hexamethylenetetramin root root
N, 1, Ring, Ring1, Ring, Ring2, C, 2, N, 3, Ring, Ring3, C, 4, N, 5, (, x, C, 6, N, 7, (, x, C, 8, Ring, Ri
ng1, ) , x, C, 10, Ring, Ring3, ) , x, C, 9, Ring, Ring2
pentamethylenetetramine|pentamethylenetetramin root root N12CNCN(CNC1)C2, x
fulvalene|fulvalen root root
c, 2, Ring, Ring1, (, x, c, 3, c, 4, c, 5, c, 1, Ring, Ring1, ) =, x, c, 2', Ring, Ring2, c, 3', c, 4', =, x
, c, 5', c, 1', Ring, Ring2
tetrathiafulvalene|tetrathiafulvalen root root
C, 2, Ring, Ring1, (, x, S, 3, C, 4, =, x, C, 5, S, 1, Ring, Ring1, ) =, x, C, 2', Ring, Ring2, S, 3', C, 4'
, =, x, C, 5', S, 1', Ring, Ring2
tetraselenafulvalene|tetrathiafulvalen root root
C, 2, Ring, Ring1, (, x, [Se], 3, C, 4, =, x, C, 5, [Se], 1, Ring, Ring1, ) =, x, C, 2', Ring, Ring2, [Se
], 3', C, 4', =, x, C, 5', [Se], 1', Ring, Ring2
labd root natural
C, 1, Ring, Ring1, C, 2, C, 3, [C@@], 4, (, x, C, 18, ) , x, (, x, C, 19, ) , x, [C@@], 5, ([H]) , x, Ring, Ri
ng2, C, 6, C, 7, [C@], 8 | a-r, (, x, C, 17, ) , x, [C@@], 9 | a-
b, (, x, [C@], 10, Ring, Ring2, Ring, Ring1, C, 20, ) , x, C, 11 | a-
t, C, 12, [C@], 13, (, x, C, 16, ) , x, C, 14, C, 15
ambros root natural C, 2, Ring, Ring1, C, 3, C, 4, [C@@], 5 | a-
b, Ring, Ring2, (, x, C, 15, ) , x, C, 6 | a-
r, [C@], 7, (, x, C, 11, (, x, C, 12, ) , x, C, 13, ) , x, C, 8, C, 9, [C@], 10, (, x, C, 14, ) , x, [C@@], 1 | a-
t, ([H]) , x, Ring, Ring2, Ring, Ring1
cedr root natural [C@@], 2, Ring, Ring1, (, x, C, 12, ) , x, C, 3, C, 4, [C@], 5 | a-
b, ([H]) , x, Ring, Ring2, [C@@], 6 | a-
r, (, x, C, 13, ) , x, (, x, C, 14, ) , x, [C@], 7, (, x, C, 11, Ring, Ring3, ) , x, [C@], 8, (, x, C, 15, ) , x, C
, 9, C, 10, [C@@], 1 | a-t, Ring, Ring1, Ring, Ring2, Ring, Ring3
cedrol root natural OC1(C)C3CC2(C(C3(C)C)CCC2C)CC1, x
apotrichothec root natural
O, 1, Ring, Ring1, [C@], 12, Ring, Ring2, (, x, C, 13, ) , x, C, 2, C, 3, C, 4, [C@@], 5 | a-
r, (, x, C, 14, ) , x, Ring, Ring2, [C@], 6 | a-
b, (, x, C, 15, ) , x, Ring, Ring3, C, 7, C, 8, C, 9, (, x, C, 16, ) , x, C, 10, [C@], 11 | a-
t, ([H]) , x, Ring, Ring3, Ring, Ring1

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germacr root natural
C,1, Ring, Ring1, C, 2, C, 3, [C@], 4, (, x, C, 15, ), x, C, 5, C, 6, [C@], 7, (, x, C, 11, (, x, C, 12, ), x,
C, 13, ), x, C, 8, C, 9, [C@@], 10, (, x, C, 14, ), x, Ring, Ring1
podocarpa|podocarp root steroid
C,1, Ring, Ring1, C, 2, C, 3, [C@@], 4, (, x, C, 15|18, ), x, (, x, C, 16|19, ), x, C, 5, Ring, Ring2, C,
6, C, 7, C, 8, Ring, Ring3, C, 14, C, 13, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, (, x, C, 17, ), x, Ri
ng, Ring1, Ring, Ring2
palustr root natural
C, x, Ring, Ring4, ., x, CC(C)C(CC3)=CC2=C3[C@]1(C)C(CC2)[C@@], x, Ring, Ring4, (C)CCC1, x
gedun root natural
C,1, Ring, Ring1, C, 2, C, 3, C, 4, (, x, C, 30, ), x, (, x, C, 31, ), x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8,
Ring, Ring3, (, x, C, x, ), x, C, 14, Ring, Ring4, C, 15, C, 16, O, x, C, 17, (, x, C, 20, Ring, Ring5, C,
x, O, x, C, 23, C, 22, Ring, Ring5, ), x, C, 13, Ring, Ring4, (, x, C, 18, ), x, C, 12, C, 11, C, 9, Ring, R
ing3, C, 10, (, x, C, 19, ), x, Ring, Ring2, Ring, Ring1
eudesm root natural
C,1, Ring, Ring1, C, 2, C, 3, [C@], 4, (C), x, [C@@], 5, ([H]), x, Ring, Ring2, C, 6, [C@], 7|a-
r, (, x, C, 11, (C), x, C, x, ), x, C, 8|a-b, C, 9|a-t, [C@], 10, (C), x, Ring, Ring2, Ring, Ring1
trichotheca|trichothec root natural C,3, Ring, Ring1, C, 4, [C@@], 5|a-
r, (, x, C, 14, ), x, Ring, Ring2, [C@], 6|a-
b, (, x, C, 15, ), x, Ring, Ring3, C, 7, C, 8, [C@], 9, (, x, C, 10, [C@], 11|a-
t, ([H]), x, Ring, Ring3, O, 1, [C@], 2, Ring, Ring1, [C@], 12, Ring, Ring2, C, 13, ), x, C, 16
scirpenol root natural [C@], 3, (O), x, Ring, Ring1, C, 4, [C@@], 5|a-
r, (, x, C, 14, ), x, Ring, Ring2, [C@], 6|a-
b, (, x, C, 15, ), x, Ring, Ring3, C, 7, C, 8, C, 9, (=, x, C, 10, [C@], 11, ([H]), x, Ring, Ring3, O, 1, [
C@], 2, Ring, Ring1, [C@@], 12, Ring, Ring2, (, x, O, x, Ring, Ring4, ), x, C, 13, Ring, Ring4, ), x,
C, 16
prosta|prost root natural C,1, C, 2, C, 3, C, 4, C, 5, C, 6, C, 7, [C@@H], 8|a-
t, (, x, C, 9, C, 10, C, 11, Ring, Ring1, ), x, [C@H], 12|a-b, Ring, Ring1, C, 13|a-
r, C, 14, C, 15, C, 16, C, 17, C, 18, C, 19, C, 20
phorbol root natural O, x, [C@@], 13, 1(, x, [C@@H], 12, 2O) [C@H] ([C@@] (C=C, a-
t, Ring, Ring3, CO) ([H]) [C@@] (O) ([C@@] (C=C(C)C4=O) ([H]), x, [C@], 4|a-b, 4(O)C, a-
r, 3) [C@@H] 2C) [C@@] 1(C)C, x
tigli|tiglia root natural
C,13, Ring, Ring1, (, x, C, 12, Ring, Ring2, ), x, [C@H], x, (, x, [C@@], 8, (, x, C, 7, =, x, C, 6|a-
t, Ring, Ring3, C, 20, ), x, ([H]), x, C, 9, (, x, [C@@], 10, (, x, C, 1, C, 2, (C), x, C, 3, Ring, Ring4,
), x, ([H]), x, C, 4|a-b, Ring, Ring4, C, 5|a-
r, Ring, Ring3, ), x, [C@@H], x, Ring, Ring2, C, x, ), x, [C@@], x, Ring, Ring1, (C), x, C, x
glutathionereduced root root
O=C(NCC(, x, O, 1@x, )=O)C(C, x, S, s, )NC(CCC(N)C(, x, O, 1@x, )=O)=O, x
glutathione root root
O=C(NCC(O)=O) [C@H] (CSSC[C@H] (NC(CC[C@H] (N)C(O)=O)=O)C(NCC(O)=O)=O)NC(CC[C@H] (N)C
(O)=O)=O, x
sphingosin|sphingosine|dihydrosphingosin|dihydrosphingosine pseudosugar unknown
x, x
sphingosin|sphingosine root root
O, x, C, 1, C, 2, (, x, N, n, ), x, C, 3, (O), x, C, 4, =, x, C, 5, C, 6, C, 7, C, 8, C, 9, C, 10, C, 11, C, 12, C, 1
3, C, 14, C, 15, C, 16, C, 17, C, 18
dihydrosphingosin|dihydrosphingosine root root
O, x, C, 1, C, 2, (, x, N, x, ), x, C, 3, (O), x, C, 4, C, 5, C, 6, C, 7, C, 8, C, 9, C, 10, C, 11, C, 12, C, 13, C,
14, C, 15, C, 16, C, 17, C, 18
phenacetin root root CCOC1=CC=C(NC(C)=O)C=C1, x
xanthotoxin root root COC1=C(OC3=O)C(C=C3)=CC2=C1OC=C2, x
troxonium root root O=C(C1=CC(OC)=C(C(OC)=C1)OC)OCC[N+] (CC) (CC)CC, x
triclopyr root root O, 1@x, C(=O)COC(N=C(C1)C(C1)=C1)=C1C1, x
thonzonium|tonzonium root root
COC1=CC=C(C=C1)CN(C2=NC=CC=N2)CC[N+] (C) (C)CCCCCCCCCCCCCCCC, x
tolonium root root NC1=CC2=C(N=C(C=C3)C(S2)=CC3=[N+] (C)C)C=C1C, x

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tolazoline root root C(c1ccccc1)C2=NCCN2,x
tiodonium root root ClC(C=C2)=CC=C2[I+]C1=CC=CS1,x
tiemonium root root C[N+](CCC(C2=CC=CC=C2)(C3=CC=CS3)O)CCOCC1,x
tiametonium root root CC[N+](C)(CCSCC[N+](C)(CC)C)C,x
tibezoneium root root
CC[N+](CC)(C)CCSC2=NC1=C(N=C(C4=CC=C(C=C4)SC3=CC=CC=C3)C2)C=CC=C1,x
tetramisole root root ClCSC2=NC(c3cccc3)CN12,x
suxethonium root root CC[N+](C)(CCOC(CCC(OCC[N+](C)(CC)C)=O)=O)C,x
suxamethonium|succinylcholine root root
C[N+](C)(CCOC(CCC(OCC[N+](C)(C)C)=O)=O)C,x
sultroponium root root C[N+](C2CCC1CC(OC(C(C3=CC=CC=C3)CO)=O)C2)CCCS([O-])(=O)=O,x
stilonium root root CC[N+](CC)(CCOC2=CC=C(C=C2)C=CC1=CC=CC=C1)CC,x
spiropentane root root
C,1, Ring, Ring1, C, 2, C, 3, Ring, Ring1, Ring, Ring2, C, 4, C, 5, Ring, Ring2
sorbitane|sorbitan root root O[C@@H]([C@@H]1[C@H](O)[C@@H](O)CO1)CO,x
sesamol root root OC1=CC(OC2)=C2C=C1,x
sepazonium root root
ClC1=CC(C1)=C(COC(C4=CC=C(C=C4Cl)Cl)CN2C=C[N+](CCC3=CC=CC=C3)=C2)C=C1,x
scopoletin root root olc(=O)ccc2cc(OC)c(O)cc12,x
salbutamol root root CC(C)(NCC(C1=CC(CO)=C(O)C=C1)O)C,x
saccharin|glucarin|saccharine|glucarine root root C(=O)1NS(=O)(=O)c2cccc21,x
saccharide|saccharinate root root C(=O)1[N-]S(=O)(=O)c2cccc21,x
imazethapyr|pursuit root root
O=C1NC(C2=C(C(,x,O,1@x,)=O)C=C(CC)C=N2)=NC1(C)C(C)C,x
pyridoxine|pyridoxin root root CC1=NC=C(CO)C(CO)=C1O,x
prolonium|hydroxytriethonium root root C[N+](C)(C)CC(O)C[N+](C)(C)C,x
prodeconium root root CCCOC(C[N+](C)(CCCCCCCCCCCCOCC[N+](C)(CC(OCCC)=O)C)C)=O,x
procaine root root Nc1ccc(C(OCCN(CC)CC)=O)cc1,x
procainamide|procaineamide root root Nc1ccc(C(NCCN(CC)CC)=O)cc1,x
pirdonium root root CC1=CC=C(C(C3=CC=CC=C3)OCC2CCCC[N+](2)C)C=C1,x
pentolonium|pentolinium root root C[N+](CCCC[N+](2)C)CCCC2)CCCC1,x
lytensium|penthonium|pentamethonium root root C[N+](C)(C)CCCC[N+](C)(C)C,x
penoctonium root root O=C(OCC[N+](CC)(CC)CCCCCCC)C(C2CCCC2)C1CCCC1,x
acetaminophen|paracetamol root root O=C(NC(C=C1)=CC=C1O)C,x
amiben|chloramben root root O,1@x,C(=O)C1=C(C1)C(N)=CC(C1)=C1,x
chlorfenac root root O,1@x,C(=O)CC(C(C1)=CC=C1Cl)=C1Cl,x
actinonin root root OCC1N(C(C(C(C)C)NC(C(CC(NO)=O)CCCC)=O)=O)CCC1,x
aminopropylon root root O=C1N(c2cccc2)N(C)C(C)=C1NC(C(C)N(C)C)=O,x
azamethonium root root CC[N+](C)(C)CCN(C)CC[N+](C)(C)CC,x
benzathonium|benzethonium root root
CC(C)(C1=CC=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
methylbenzathonium|methylbenzethonium root root
CC(C)(C1=CC(C)=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
benzilonium root root O=C(OC1C[N+](CC)(CC1)CC)C(C2=CC=CC=C2)(C3=CC=CC=C3)O,x
bevonium root root OC(C(OCC3[N+](C)(C)CCCC3)=O)(C2=CC=CC=C2)C1=CC=CC=C1,x
carpronium root root COC(CCC[N+](C)(C)C)=O,x
carvone root root CC(C1=O)=CCC(C1)C(C)=C,x
cetrimonium root root CCCCCCCCCCCCCCCCCC[N+](C)(C)C,x
chloraminophen root root ClCCN(C1=CC=C(CCCC(O)=O)C=C1)CCC1,x
chloraminophenamide root root O=S(N)(C1=C(C1)C=C(N)C(S(=O)(N)=O)=O,x
chloramphenicol root root OC[C@@H](NC(C(C1)C1)=O)[C@@H](C1=CC=C([N+])([O-])(=O)C=C1)O,x
chlorphonium root root CCCC[P+](CCCC)(CCCC)CC1=CC=CC=C1,x
ciclonium root root CC[N+](CC)(CCOC(C1CC2CC1C=C2)(C3=CC=CC=C3)C)C,x
cyclopyrronium root root CC[N+](CCC(OC(C(C3=CC=CC=C3)C2CCCC2)=O)C1)C,x
cypion root root CCCCC1CCCC1,x

decamethonium root root C[N+] (C) (C) CCCCCCCCCC[N+] (C) (C) C, x
deditionium root root
CC (C1=CC=C (C=C1OCC[N+] (C) (CCCCCCCCC[N+] (C) (CCOC2=CC (C) =CC=C2C (C) C) C) C) C) C, x
denatonium root root CC[N+] (CC (NC (C (C) =CC=C2) =C2C) =O) (CC) CC1=CC=CC=C1, x
dicyclopentadiene root root
C, 1, Ring, Ring1, c, 2, c, 3, C, 3a, Ring, Ring2, C, 4, Ring, Ring3, c, 5, c, 6, C, 7, (, x, C, x, Ring, R
ing3,), x, C, 7a, Ring, Ring2, Ring, Ring1
dimecolonium root root CC1CCCC ([N+] 1 (C) C) C (OCC[N+] (C) (C) C) =O, x
dimidium root root c1cc (N) cc2c (c3cccc3) [n+] (C) c4cc (N) ccc4c21, x
dinoseb root root CC (C=C (C ([N+] ([O-]) =O) C=C1 [N+] ([O-]) =O) =C1O) CC, x
disilethylene root root [Si], 1, C, 2, C, 3, [Si], 4
disiquonium root root C[N+] (CCCCCCCCC) (CCC[Si] (OC) (OC) OC) CCCCCCCCCC, x
doteфонium root root CN (C (C (C2=CC=CC=C2) (C3=CC=CC=C3) O) =O) CC [N+] 1 (CCCC1) C, x
ebdc root root S, 1@x, C (NCCNC (, x, S, 1@x,) =S) =S, x
edrophonium root root CC[N+] (C) (C1=CC=CC (O) =C1) C, x
emepronium root root CC[N+] (C) (C (CC (C2=CC=CC=C2) C1=CC=CC=C1) C) C, x
fentonium root root
C[N+] 3 (C4CCC3CC (OC (C (C5=CC=CC=C5) CO) =O) C4) CC (C1=CC=C (C2=CC=CC=C2) C=C1) =O, x
fludazonium root root
O=C (C1=CC=C (F) C=C1) CN (C=C2) C= [N+] 2CC (C4=C (C=C (C=C4) C1) C1) OCC3=C (C=C (C=C3) C1) C1, x
furacrin loveracid root CC1=CC (C=C2C (C (CC) =C) =O) =C (C=C2C) O1, x
fosamine|fosamin root root O=P (O) (OCC) C (N) =O, x
fubrogonium root root CC[N+] (CC) (CCC (OC (C1=CC=C (O1) Br) =O) C) C, x
furtrethonium root root C[N+] (C) (C) CC1=CC=CC1, x
glufosinate|glufosinat root root CP (O) (CCC (C (, x, O, 1@x,) =O) N) =O, x
glycopyrronium root root OC (C1CCCC1) (C2=CC=CC=C2) C (OC (CC3) C [N+] 3 (C) C) =O, x
glyphosate|glyphosat root root O, 1@x, C (CNCP (O) (O) =O) =O, x
heteronium root root C[N+] 1 (CCC (OC (C (C2=CC=CC=C2) (C3=CC=CC=C3) O) =O) C1) C, x
hexafluoronium root root
C[N+] (C) (C2C1=C (C3=C2C=CC=C3) C=CC=C1) CCCCCC[N+] (C) (C6C4=C (C5=CC=CC=C5) C=CC=C4) C
, x
hexamethonium root root C[N+] (C) (CCCCCC[N+] (C) (C) C) C, x
hexasonium root root C[S+] (CCOC (C (C2=CC=CC=C2) C1CCCCC1) =O) C, x
hexopyrronium root root C[N+] 1 (CCC (OC (C (C2CCCC2) (C3=CC=CC=C3) O) =O) C1) C, x
imazaquin root root CC (C1 (N=C (C3=NC2=CC=CC=C2C=C3C (, x, O, 1@x,) =O) NC1=O) C) C, x
isoluminol root root NC1=CC=C2C (C (MNC2=O) =O) =C1, x
mebezonium root root C[N+] (C) (C1CCC (CC2CCC ([N+] (C) (C) C) CC2) CC1) C, x
mecetronium root root CCCCCCCCCCCCCCCCCC[N+] (C) (CC) C, x
chloramben root root O, 1@x, C (=O) C1=C (N) C (C1) =CC (C1) =C1, x
nitronium root root O=[N+] =O, x
nifuroxime root root ON=Cc1ccc (o1) [N+] (=O) [O-], x
octaфонium root root CC[N+] (CCOC1=CC=C (C=C1) CC (C) (CC (C) C) C) (CC2=CC=CC=C2) CC, x
otilonium root root
CCCCCCCCOC1=CC=CC=C1C (NC2=CC=C (C (OCC[N+] (CC) (CC) C) =O) C=C2) =O, x
oxiteфонium root root CC[N+] (CC) (CCOC (C (C1=CC=CC=C1) (C2=CC=CC=C2) O) =O) C, x
pxydipentonium root root C[NH+] (CCCCCOCOC[N+] (C) (C) C) C, x
oxyphenonium root root CC[N+] (CC) (CCOC (C (C1CCCCC1) (C2=CC=CC=C2) O) =O) C, x
oxyppyrronium root root C[N+] 1 (CCCC1COC (C (C2CCCC2) (C3=CC=CC=C3) O) =O) C, x
oxysonium root root C[S+] (CCOC (C (C1CCCCC1) (C2=CC=CC=C2) O) =O) C, x
amezinium root root COC1=CC (N) =CN= [N+] 1C2=CC=CC=C2, x
amenzpyrinium root root CN (C (OC1=CC=C [N+] (CC2=CC=CC=C2) =C1) =O) C, x
carcainium root root C[N+] (CC (NC1=CC=CC=C1) =O) (CC (NC2=CC=CC=C2) =O) C, x
clonidine root root
c, p, Ring, Ring1, c, m, c, x, (C1), x, c, x, (NC2=NCCN2), x, c, x, (C1), x, c, x, Ring, Ring1
dequalinium root root
CC1=CC (N) =C2C (C=CC=C2) = [N+] 1CCCCCCCCC[N+] (C (C) =C3) =C (C=CC=C4) C4=C3N, x
elliptinium root root CC (C2=C1C=C [N+] (C) =C2) =C (C3=C4C=CC (O) =C3) C (N4) =C1C, x

fazadinium root root
CC5=C(N(C6=[N+]5C=CC=C6)N=NN3C(C2=CC=CC=C2)=C([N+]4=C3C=CC=C4)C)C1=CC=CC=C1,x
fenpiverinium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C(N)=O)CCCCC1,x
methanthelinium root root O=C(C2C3=C(C=CC=C3)OC1=CC=CC=C12)OCC[N+](CC)(C)CC,x
methylthioninium root root CN(C1=CC([S+]=C(C=C(N(C)C)C=C3)C3=N2)=C2C=C1)C,x
metocinium root root C[N+](C)(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)C,x
nicotine root root CN1C(C2=CC=CN=C2)CCCC1,x
nolinium root root ClC(C=C3)=C(C1)C=C3NC2=CC1=CC=CC=[N+]1C=C2,x
pentolinium root root C[N+](CCCC[N+](C)CCCC2)CCCC1,x
prifinium root root CC[N+](CCC(C2C)=C(C3=CC=CC=C3)C1=CC=CC=C1)CC,x
promethazine root root CC(N(C)C)CN1C3=C(C=CC=C3)SC2=C1C=CC=C2,x
pyrvinium root root
CN(C1=CC4=C([N+](C)=C(C=C4)C=CC2=C(C)N(C3=CC=CC=C3)C(C)=C2)C=C1)C,x
rosaniline|rosanilin root root
N=C(C=C3)C=CC3=C(C2=CC=C(N)C(C)=C2)C1=CC=C(N)C=C1,x
senfol root root N=C=S,x
tartrazine root root O=C1N(C3=CC=C([S](=O)([O-])=O)C=C3)N=C(C([O-])=O)C1N=NC2=CC=C([S](=O)([O-])=O)C=C2.[Na+].[Na+].[Na+],x
thonzylaminium root root COC2CC(CC2)CN(C1CCCC1)CC[N+](C)C,x
trantelinium root root C[N+]1(C2CCC1CC(OC(C4C3=CC=CC=C3OC5=C4C=CC=C5)=O)C2)C,x
trimethidinium root root CC1(C2CCC1(C[N+](CCC[N+](C)(C)C)(C2)C)C)C,x
thenium root root C[N+](CCOC2=CC=CC=C2)(C)CC1=CC=CS1,x
menrium|tropium|librium|solium root root [O-][N+](CC(NC)=N3)=C(C2=C3C=CC(C1)=C2)C1=CC=CC=C1,x
oxapropanium root root C[N+](C)(C)CC1OCOC1,x
furium root root [O-][N+](C1=CC=C(C2=CSC(NC(C)=O)=N2)O1)=O,x
tropylium root root C1=CC=C[C+]C=C1,x
acetaminophen root root Oc1ccc(cc1)NC(=O)C,x
acetur root root CCNC(=O)C,x
afurololol root root CC(C)(NCC(COC(C=CC=C1CO2)=C1C2=O)O)C,x
agallol root root COCC[Hg]Cl,x
alizarin root root O=C(c2cccc23)c1c(O)c(O)ccc1C3=O,x
allantoin root root O=C(N1)NC(NC(N)=O)C1=O,x
amantanum root root CCCCCCCC[N+](C)(CCOC(C23CC1CC(C3)CC(C2)C1)=O)C,x
aminopentamide root root CC(N(C)C)CC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=O,x
amprolium root root CCCC2=NC=C(C(N)=N2)C[N+]1=C(C)C=CC=C1,x
aporph root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, C, 4, C, 5, N, 6, (C), x, C, 6a, Ring, Ring3, C, 7, c, 7
a, Ring, Ring4, c, 8, c, 9, c, 10, c, 11, c, 11a, Ring, Ring4, c, 11b, Ring, Ring1, c, 11c, Ring, Ring
2, Ring, Ring3
noraporph root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, C, 4, C, 5, N, 6, C, 6a, Ring, Ring3, C, 7, c, 7a, Ring
, Ring4, c, 8, c, 9, c, 10, c, 11, c, 11a, Ring, Ring4, c, 11b, Ring, Ring1, c, 11c, Ring, Ring2, Ring
, Ring3
aspirin root root O=C(O)c1cccc1OC(C)=O,x
azaspirium root root
COC(C1=C(C(OC)=C23)C=COC1)=C3OC5=C(C[N+]4(CCC5=C)CCCC4)C2=O,x
bephenium root root C[N+](CCOC1=CC=CC=C1)(CC2=CC=CC=C2)C,x
berb root root c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, C, 5, C, 6, N, 7 |a-
r, Ring, Ring3, C, 8, c, 8a, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring4, C, 13 |a-
t, C, 13a |a-b, Ring, Ring3, c, 13b, Ring, Ring2, Ring, Ring1
bidimazium root root
CN(C1=CC=C(C=CC2=[N+](C)C(C3=CC=C(C4=CC=CC=C4)C=C3)=CS2)C=C1)C,x
bretylium root root CC[N+](C)(CC1=C(Br)C=CC=C1)C,x
busulfan root root O=S(OCCCCOS(=O)(C)=O)(C)=O,x
carazolol root root OC(CNC(C)C)COC1=CC=CC2=C1C(C=CC=C3)=C3N2,x
clofilium root root CCCCCCC[N+](CC)(CCCCC1=CC=C(C=C1)C1)CC,x

datelliptium root root
CC1=C4C(C=C[N+](CC[NH+](CC)CC)=C4)=C(C)C3=C1C2=C(N3)C=CC(O)=C2,x
demecarium root root
CN(C(OC2=CC=CC([N+](C)(C)C)=C2)=O)CCCCCCCCCN(C(OC1=CC=CC([N+](C)(C)C)=C1)=O)C,x
dibromantin root root CC(C(N1Br)=O)(N(Br)C1=O)C,x
digermin root root O=[N+](O-)]C1=CC(C(F)(F)F)=CC([N+](O-))=O=C1N(CCC)CCC,x
diphenhydramine root root CN(C)CCOC(C2=CC=CC=C2)C1=CC=CC=C1,x
dithizone root root S=C(NNC2=CC=CC=C2)N=NC1=CC=CC=C1,x
dopamine root root
NCC,x,c,1, Ring, Ring1, c, 2, c, 3, (O), x, c, 4, (O), x, c, 5, c, 6, Ring, Ring1
etipirium root root C[N+](CCOC(C(C2=CC=CC=C2)(C3=CC=CC=C3)O)=O)CCCC1,x
fench root root
C, 2 | a | alpha, Ring, Ring1, c, 3, (C)(C), x, c, 4, (, x, c, 5, c, 6, c, 1, Ring, Ring2, (C), x, Ring, Ring1,) , x, c, 7, Ring, Ring2
feniodium root root ClC2=CC=C(C(C1)=C2)[I+]C1=CC=C(C=C1C1)C1,x
flutropium root root C[N+](C2CCC1CC(OC(C(C3=CC=CC=C3)(C4=CC=CC=C4)O)=O)C2)CCF,x
furazolium root root [O-][N+](C1=CC=C(C2=CSC3=[N+]2CCN3)O1)=O,x
halopenium root root CC(C1=CC(C1)=C(C=C1OCCC[N+](C)(CC2=CC=C(C=C2)Br)C)C)C,x
hexafluorenium root root
C[N+](C)(C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCC[N+](C)(C6C4=C(C5=CC=CC=C56)C=CC=C4)C,x
hexocyclium root root C[N+](CCN(CC(C2CCCC2)(C3=CC=CC=C3)O)CC1)C,x
ethidium|homidium root root
NC(C=C3)=CC2=C3C1=CC=C(N)C=C1C(C4=CC=CC=C4)=[N+]2CC,x
indenolol root root CC(NCC(COC2=C1C=CCC1=CC=C2)O)C,x
ionone|ionon|alphaionon|alphaionone root root O=C(C)C=CC1c(C)CCCC1(C)C,x
betaionone|betaionon root root O=C(C)C=CC1=C(C)CCCC1(C)C,x
isometamidium root root
CC[N+](C2=C(C5=CC=C(C=C45)N)C=CC(NN=NC3=CC=CC(C(N)=N)=C3)=C2)C1=CC=CC=C1,x
isophor root root C, 1, Ring, Ring1, c, 2, c, 3, (C), x, c, 4, c, 5, (C)(C), x, c, 6, Ring, Ring1
isophorone root root
O=, x, c, 1, Ring, Ring1, c, 2, =, x, c, 3, (C), x, c, 4, c, 5, (C)(C), x, c, 6, Ring, Ring1
lapirium root root O=C(NCCOC(CCCCCCCCCC)=O)C[N+](C)=CC=CC=C1,x
methylbenactyzium root root OC(C1=CC=CC=C1)(C2=CC=CC=C2)C(OC[C[N+](CC)(C)CC]=O,x
benactyzine root root CCN(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)CC,x
miripirium root root CCCCCCCCCCCCC[N+](C)=CC=C(C)C=C1,x
neopentylglycol root root OCC(C)(C)CO,x
nioxime root root ON=C(CCCC1)C1=NO,x
oxapium root root C[N+](C2COC(C3CCCC3)(C4=CC=CC=C4)O2)CCCCC1,x
oxolin root root CC2=CN(CC)C1=CC(OC3)=C3C=C1C2=O,x
oxprenolol root root CC(NCC(COC1=CC=CC=C1OCC=C)O)C,x
oxybenzone root root O=C(C1=CC=CC=C1)C(C=CC(OC)=C2)=C2O,x
penbutolol root root OC(CNC(C)(C)C)COC1=C(C2CCCC2)C=CC=C1,x
pentacynium root root
C[N+](CCCC(C1=CC=CC=C1)(C2=CC=CC=C2)C#N)(CC[N+](C3(COCC3)C)C)C,x
pentazocine root root CC2C3(C)C1=CC(O)=CC=C1CC2N(CC=C(C)C)CC3,x
phenacetur root root CCNC(=O)Cc1cccc1,x
phencyclidine|angeldust root root c1(C2(N3CCCC3)CCCC2)cccc1,x
pinaverium root root COC4=CC(Br)=C(C=C4OC)C[N+](C3(COCC3)CCOCC1CCC2CC1C2(C)C,x
piperylene root root C=CC=CC,x
piroctanylium root root CC(C)CCCC(C)CC[N+](C)=CC=CC1,x
pirocurarium root root CC[N+](CC)(CCOCCOC(C([N+](C2(CCCCC2)C)C1=CC=CC=C1)=O)C,x
pranolium root root CC(C)[N+](C)(C)CC(O)COC1=C2C(C=CC=C2)=CC=C1,x
pretamazium root root
CC[N+](C3=C(SC=C3C4=CC=C(C5=CC=CC=C5)C=C4)C=CC1=CC=C(N2CCCC2)C=C1,x
propanolol root root OC(CNC(C)C)COC1=C2C(C=CC=C2)=CC=C1,x

propidium root root
C[N+](CC)(CC)CCC[N+](C3=C2C=CC(N)=C3)=C(C4=CC=CC=C4)C1=C2C=CC(N)=C1,x
prospidium root root C1CC(O)CN3CC[N+](C3)CC[N+](C2)CCN(CC1)CC(O)CC1,x
pyritidium root root
CC1=CC(NC2=CC(C(C3=CC=C(C=C3)N)=[N+](C5=CC(N)=CC=C45)C)=C4C=C2)=NC(N)=[N+](C)1C,x
quinomethionate|chinomethionate root root O=C3SC2=NC1=CC(C)=CC=C1N=C2S3,x
salicin root root O[C@H]1O[C@@H](OC2=CC=CC=C2CO)[C@H](O)[C@@H](O)[C@H]1O,x
serenium root root CCOC(C=C2)=CC=C2N=NC1=CC=C(N)C=C1N,x
sintropium root root CCCC(C(OC1CC2CCC([N+](C2)C(C)C)C1)=O)CCC,x
stilbazium root root
CC[N+](C1=C(C=CC5=CC=C(C=C5)N4CCCC4)C=CC=C1C=CC3=CC=C(C=C3)N2CCCC2,x
timepidium root root COC2CC(C[N+](C)(C2)C)=C(C3=CC=CC=C3)C1=CC=CC=C1,x
tipetropium root root CCC[N+](C1(C2CCC1CC(OC4C3=CC=CC=C3CSC5=CC=CC=C45)C2)C,x
tiquizium root root C[N+](C13CCCC1CCC(C3)=C(C4=CC=CC=C4)C2=CC=CC=C2,x
trimethylsilyldifluoride root root [Si-](C)(C)(C)(F)F,x
tricine root root OCC(CO)(CO)NCC(O)=O,x
toliodium root root CC2=CC=C(C=C2)[I+](C1=CC=C(C=C1)C,x
trazium root root OC1(C4=CC=C(C=C4)C1)NC=N[N+](C1)C2=CC=CC=C2C=C3,x
trepirium root root C[N+](C)(CCOC(C1CCC[N+](C1)C)=O)C,x
tropolone|tropalone root root
O,x,c,1, Ring, Ring1, c, 7, c, 6, c, 5, c, 4, c, 3, c, 2, Ring, Ring1, 0,x
tyloxapol root root NCCc1ccc(O)cc1,x
urocan root root
C,x,C,a|alpha,=,x,C,b|beta,c,4, Ring, Ring1, n, 3, c, 2, n, 1|prefhydro,c,5, Ring, Ring1
verbenone root root O=C1C(C2)C(C)(C)C2C(C)=C1,x
yohimb|yohimbin loveracid root C,x, Ring, Ring6, ., x, N, 1|a-
r, Ring, Ring1, c, 2, Ring, Ring2, [C@], 3, ([H]), x, Ring, Ring3, N, 4, (, x, c, 5, c, 6, c, 7, =, x, Ri
ng, Ring2, c, 8|a-t, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 13|a-
b, Ring, Ring4, Ring, Ring1,) , x, c, 21, [C@@], 20, ([H]), x, Ring, Ring5, c, 19, c, 18, [C@H], 17,
(O), x, [C@H], 16, Ring, Ring6, [C@], 15, ([H]), x, Ring, Ring5, c, 14, Ring, Ring3
yohimb|yohimba root root N, 1|a-
r, Ring, Ring1, c, 2, Ring, Ring2, [C@], 3, ([H]), x, Ring, Ring3, N, 4, (, x, c, 5, c, 6, c, 7, =, x, Ri
ng, Ring2, c, 8|a-t, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 13|a-
b, Ring, Ring4, Ring, Ring1,) , x, c, 21, [C@@], 20, ([H]), x, Ring, Ring5, c, 19, c, 18, c, 17, c, 16
, [C@], 15, ([H]), x, Ring, Ring5, c, 14, Ring, Ring3
yohimbine|yohimbin root root N, 1|a-
r, Ring, Ring1, c, 2, Ring, Ring2, [C@], 3, ([H]), x, Ring, Ring3, N, 4, (, x, c, 5, c, 6, c, 7, =, x, Ri
ng, Ring2, c, 8|a-t, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 13|a-
b, Ring, Ring4, Ring, Ring1,) , x, c, 21, [C@@], 20, ([H]), x, Ring, Ring5, c, 19, c, 18, [C@H], 17,
(O), x, [C@H], 16, (C(=O)OC), x, [C@], 15, ([H]), x, Ring, Ring5, c, 14, Ring, Ring3
oxayohimb|oxayohimba root root N, 1|a-
r, Ring, Ring1, c, 2, Ring, Ring2, [C@], 3, ([H]), x, Ring, Ring3, N, 4, (, x, c, 5, c, 6, c, 7, =, x, Ri
ng, Ring2, c, 8|a-t, Ring, Ring4, c, 9, c, 10, c, 11, c, 12, c, 13|a-
b, Ring, Ring4, Ring, Ring1,) , x, c, 21, [C@@], 20, ([H]), x, Ring, Ring5, c, 19, c, 18, O, 17, c, 16
, [C@], 15, ([H]), x, Ring, Ring5, c, 14, Ring, Ring3
morphinan root natural c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 12|a-t, Ring, Ring2, [C@], 13|a-
b, Ring, Ring4, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, [C@@], 14, Ring, Ring3, ([H]), x, [C@], 9|a-
r, (, x, N, 17, c, 16, c, 15, Ring, Ring4,) , x, c, 10, c, 11, Ring, Ring2, Ring, Ring1
morphine root natural
c, 1, Ring, Ring1, c, 2, c, 3, (O), x, c, 4, (, x, O, x, Ring, Ring5,) , x, c, 12|a-
t, Ring, Ring2, [C@], 13|a-
b, Ring, Ring4, Ring, Ring3, c, 5, Ring, Ring5, [C@@], 6, (O), x, c, 7, =, x, c, 8, [C@@], 14, Ring, R
ing3, ([H]), x, [C@], 9|a-
r, (, x, N, 17, (C), x, c, 16, c, 15, Ring, Ring4,) , x, c, 10, c, 11, Ring, Ring2, Ring, Ring1
codeine root natural
c, 1, Ring, Ring1, c, 2, c, 3, (OC), x, c, 4, (, x, O, x, Ring, Ring5,) , x, c, 12|a-
t, Ring, Ring2, [C@], 13|a-

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b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,R
ing3,([H]),x,[C@],9|a-
r,(x,N,17,(C),x,C,16,C,15,Ring,Ring4,)x,C,10,c,11,Ring,Ring2,Ring,Ring1
codeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(x,O,x,Ring,Ring5,)x,c,12|a-
t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring
3,([H]),x,[C@],9|a-
r,(x,N,17,(C),x,C,16,C,15,Ring,Ring4,)x,C,10,c,11,Ring,Ring2,Ring,Ring1
dihydrocodeinone|hydrocodeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(x,O,x,Ring,Ring5,)x,c,12|a-
t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring
3,([H]),x,[C@],9|a-
r,(x,N,17,(C),x,C,16,C,15,Ring,Ring4,)x,C,10,c,11,Ring,Ring2,Ring,Ring1
thebacon root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(x,O,x,Ring,Ring5,)x,c,12|a-
t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(OC(=O)C),x,=,x,C,7,C,8,[C@@],14,Ring
,Ring3,([H]),x,[C@],9|a-
r,(x,N,17,(C),x,C,16,C,15,Ring,Ring4,)x,C,10,c,11,Ring,Ring2,Ring,Ring1
ergoline|ergolin root natural
n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Ring3,N,6,C,7,C,8|a-
t,C,9|a-b,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lyserg root natural
C,x,Ring,Ring5,.x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Rin
g3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lysergide root natural
C,x,Ring,Ring5,(=O)N(CC)CC.x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H])
,x,Ring,Ring3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
ergotaman root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,)x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,N,x,[
C@],2',Ring,Ring5,C,3',N,4',Ring,Ring6,C,5',C,6',N,7',Ring,Ring7,C,8',C,9',C,10'
,[C@],11',([H]),x,Ring,Ring7,[C@@H],12',Ring,Ring6,O,1',Ring,Ring5
ergocornine|ergocornin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,)x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
,12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocorninine|ergocorninin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,)x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocristine|ergocristin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4,)x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9ccc

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cc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptine|ergocryptin|ergocriptine|ergocriptin|alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|bergocryptin|bergocriptine|bergocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)CC),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptinine|ergocryptinin|ergocriptinine|ergocriptinin|alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergocryptinine|bergocryptinin|bergocriptinine|bergocriptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergosine|ergosin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergotamine|ergotamin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9cccc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 bromocryptine|bromocryptin|bromocriptine|bromocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,(Br),x,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ecgonidine|ecgonidin root root
 [C@@],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,c,x,c,x,(x,C,x,(=O),x,O,1@x),x,[C@],x,([H]),x,(x,N,x,(C),x,Ring,Ring1),x,C,x,C,x,Ring,Ring2

ecgonine|ecgonin root root
 [C@@],x,([H]),x,ring,ring1,ring,ring2,c,x,[C@H],x,(o),x,[C@H],x,(,x,c,x,(=o),x,o
 ,1@x,) ,x,[C@],x,([H]),x,(,x,n,x,(c),x,ring,ring1,) ,x,c,x,c,x,ring,ring2
 methylviologen root root
 c,1,ring,ring1,(,x,c,2,c,3,[n+],4,(c),x,c,5,c,6,ring,ring1,) ,x,c,1',ring,ring2,c
 ,2',c,3',[n+],4',(c),x,c,5',c,6',ring,ring2
 ethylviologen root root
 c,1,ring,ring1,(,x,c,2,c,3,[n+],4,(cc),x,c,5,c,6,ring,ring1,) ,x,c,1',ring,ring2,
 c,2',c,3',[n+],4',(cc),x,c,5',c,6',ring,ring2
 benzylviologen root root
 c,1,ring,ring1,(,x,c,2,c,3,[n+],4,(Cc3cccc3),x,c,5,c,6,ring,ring1,) ,x,c,1',ring
 ,ring2,c,2',c,3',[n+],4',(Cc4cccc4),x,c,5',c,6',ring,ring2
 pheneturide root root O=C(N)NC(C(C)C1=CC=CC=C1)=O,x
 lactide|dilactide root root CC(OC1=O)C(OC1C)=O,x
 gallion root root OC(C(C1)=CC([N+])([O-]
]) =O)=C3)=C3N=NC1=C(S(=O)(O)=O)C=C(C=C(S(=O)(O)=O)C=C2N)C2=C1O,x
 clofibr root root CC(C)(OC1=CC=C(C=C1)C1)C,x
 paraben root root O,1@x,C(C1=CC=C(O)C=C1)=O,x
 edetate|versenate|edta root root
 O,1@x,C(CN(CC(,x,O,1@x,)=O)CCN(CC(,x,O,1@x,)=O)CC(,x,O,1@x,)=O)=O,x
 fusar root root CC1=CC=C(CCCC)C=N1,x
 lironion root root COC1=CC=C(OC2=CC=C(C=C2)NC(N(C)C)=O)C=C1,x
 thionalide root root O=C(CS)NC2=CC1=CC=CC=C1C=C2,x
 tolperisone root root CC(C(C2=CC=C(C)C=C2)=O)CN1CCCCC1,x
 valethamate root root CCC(C(C(OC[N+](CC)(CC)C)=O)C1=CC=CC=C1)C,x
 secbutabarbitol|butalan root root O=C(N1)NC(C(C)CC)(CC)C1=O)=O,x
 furalan root root O=C(N2)N(CC2=O)N=CC1=CC=C([N+])([O-])=O)O1,x
 boc|tboc root nprotect C,4@x,(=O)OC(C)(C)C,x
 z-nprot root nprotect C,4@x,(=O)OCc1cccc1,x
 msoc root nprotect C,4@x,(=O)OCCS(=O)(=O)C,x
 cbz root nprotect
 C,4@x,(=O)OC,x,c,1,ring,ring1,=,x,c,2,c,3,=,x,c,4,c,5,=,x,c,6,ring,ring1
 fmoc root nprotect C,4@x,(=O)OCC1C2=CC=CC=C(C3=CC=CC=C13)2,x
 dansyl root nprotect S,4@x,(C2=CC=CC1=C(N(C)C)C=CC=C12)(=O)=O,x
 dabsyl root nprotect S,4@x,(c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(=O)=O,x
 bansyl root nprotect S,4@x,(C2=CC=CC1=C(N(CCCC)CCCC)C=CC=C12)(=O)=O,x
 nps root nprotect S,4@x,c1c([N+])(=O)[O-])cccc1,x
 tfa root nprotect C,4@x,(=O)C(F)(F)F,x
 acm root nprotect C,4@x,NC(=O)C,x
 phacm root nprotect C,4@x,NC(=O)Cc1cccc1,x
 creatine root root CN(C(N)=N)CC(O)=O,x
 panthenol root root CC(CO)(C(C(NCCCCO)=O)O)C,x
 alanate root root [AlH4-],x
 cyanamide root root NC#N,x
 eprolin root root CC1=C2C(OC(CCCC(C)CCCC(C)CCCC(C)C)(C)CC2)=C(C)C(C)=C1O,x
 eserine|physostigmine root root O=C(NC)OC1=CC=C(N(C)C3C2(C)CCN3C)C2=C1,x
 prolan root root CC([N+])([O-])=O)C(C2=CC=C(C1)C=C2)C1=CC=C(C1)C=C1,x
 tropanserine root root CN1C2CCC1CC(OC(C3=CC(C)=CC(C)=C3)=O)C2,x
 butanserine root root FC1=CC=C(C(C4CCN(CC4)CCCCN3C(NC2=CC=CC=C2C3=O)=O)=O)C=C1,x
 amiprol|domalium|kiatrium|levium|relanium|tensium|umbrium|velium|valium root
 root O=C1CN=C(C3=CC=CC=C3)C2=C(C=CC(C1)=C2)N1C,x
 prolate root root S=P(OC)(OC)SCN1C(C(C=CC=C2)=C2C1=O)=O,x
 adaprolol root root CC(NCC(COC4=CC=C(C=C4)CC(OC(C2)C1)=O)O)C,x
 agmatine root root NC(NCCCCN)=N,x
 algolysin root root CCC(C(C1=CC=CC=C1)(C2=CC=CC=C2)CC(C)N(C)C)=O.[H]C1,x
 altanserine root root FC1=CC=C(C(C2CCN(CC4C(NC3=CC=CC=C3C4=O)=S)CC2)=O)C=C1,x

angelicin root root
c,1, Ring, Ring1, c, 2, o, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, (=O),
x, o, 9, c, 9a, Ring, Ring3, c, 9b, Ring, Ring2, Ring, Ring1
asparagusate root root OC(C1CSSC1)=O,x
aspartame root root O=C(OC)C(NC(C(N)CC(O)=O)=O)CC1=CC=CC=C1,x
bisoprolol root root OC(CNC(C)C)COC1=CC=C(COCCOC(C)C)C=C1,x
bornaprolol root root OC(CN(CC)C)CC1=CC=CC=C1C2C3CCC(C3)C2,x
broncholysin root root OC(C(CS)NC(C)=O)=O,x
bunaprolast root root CCCCC2=C(OC(C)=O)C1=CC=CC=C1C(OC)=C2,x
butethal root root CCCCC(C(NC1=O)=O)(C(N1)=O)CC,x
capsaicin root root O=C(CCCC/C=C/C(C)C)NCc1ccc(O)c(OC)c1,x
carbachol root root C[N+](C)(C)CCOC(N)=O,x
carlsoprol root root CC(COC(N)=O)(CCC)COC(NC(C)C)=O,x
caryolysine root root ClCCN(C)CCCl,x
chloral root root O=CC(Cl)(Cl)Cl,x
chloralhydrate root root OC(O)C(Cl)(Cl)Cl,x
bromal root root O=CC(Br)(Br)Br,x
bromalhydrate root root OC(O)C(Br)(Br)Br,x
chrysanthemum|chrysanthem root root ClC(C=C(C)C)C(C)(C)1,x
celiprolol root root OC(CNC(C)(C)C)COC1=C(C(C)=O)C=C(NC(N(CC)CC)=O)C=C1,x
cinanserine root root CN(CCCSC1=CC=CC=C1NC(C=CC2=CC=CC=C2)=O)C,x
clemeprol root root CN(CC(C(C2=CC=CC(Cl)=C2)C1=CC=CC=C1)O)C,x
coumal root root Cc1ccc(=O)oc1,x
creatinine root root N1C(=N)N(C)CC(=O)1,x
cyclen root root
N,1, Ring, Ring1, C, 2, C, 3, N, 4, C, 5, C, 6, N, 7, C, 8, C, 9, N, 10, C, 11, C, 12, Ring, Ring1
cyprolidol root root OC(C3=CC=CC=C3)(C4=CC=CC=C4)C1CC1C2=CC=NC=C2,x
deprol root root CC(COC(N)=O)(CCC)COC(N)=O,x
dibuprol root root CCCCCC(O)COC(C)C,x
eburnamonine root root O=C2N(c3cccc34)C1=C4CCN5C1C(CCC5)(CC)C2,x
exaprolol root root CC(NCC(COC1=CC=CC=C1C2CCCCC2)O)C,x
epichlorohydrin root root ClCC1CO1,x
epithiochlorohydrin root root ClCC1CS1,x
epifluorohydrin root root FCC1CO1,x
epibromohydrin root root BrCC1CO1,x
erban root root O=C(CC)NC1=CC(Cl)=C(Cl)C=C1,x
ethacryn root root CCOC1=C(Cl)C(Cl)=C(C=C1)C(C(C)=O)=O,x
farmiserine|cycloserine|cycloserin|micoserina root root NC(CON1)C1=O,x
fascaplysin root root O=C(C5=C4C=CC=C5)C1=[N+]4C=CC2=C1NC3=C2C=CC=C3,x
febuprol root root CCCCCC(O)COC1=CC=CC=C1,x
fermine root root O=C(OC)C1=CC=CC=C1C(OC)=O,x
fertilysin root root O=C(C(Cl)Cl)NCCCCCCCCNC(C(Cl)Cl)=O,x
formamidinedisulfide root root NC(SSC(N)=N)=N,x
ftorafur root root O=C(N1)N(C2CCCO2)C=C(F)C1=O,x
geneserine|eseridine root root CC23C1=CC(OC(NC)=O)=CC=C1N(C)C2ON(CC3)C,x
glutim|pidol root root C,x,C,5, Ring, Ring1, C, 4, C, 3, C, 2, (=O),x,N,1, Ring, Ring1
hexethal root root O=C(N1)NC(C(CCCCC)(CC)C1=O)=O,x
ibuprofen root root C(C)(C)Cc1ccc(cc1)C(C)C(=O)O,x
indameth root root ClC(C=C3)=CC=C3C(N2C(C)=C(CC(O)=O)C1=CC(OC)=CC=C12)=O,x
iomeprol root root CN(C1=C(I)C(C(NCC(CO)O)=O)=C(I)C(C(NCC(CO)O)=O)=C1I)C(CO)=O,x
iridocin root root NC(C1=CC(CC)=NC=C1)=S,x
isatoicanhydride root root
O=C(O2)c,1, Ring, Ring1, c, 6, c, 5, c, 4, c, 3, c, 2, Ring, Ring1, NC2=O,x
isoprene root root C=CC(=C)C,x
isoxaprolol root root CC1=NOC(C=CC2=CC=CC=C2OCC(CNC(C)(C)C)O)=C1,x
ketanserine root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=O)CC2)=O)C=C1,x

limonene root root
C,7,c,1, Ring, Ring1, c,2,c,3,c,4, (,x,c,8, (=,x,c,9,), x,c,10,), x,c,5,c,6, Ring, Ring1
meprol|meproleaf root root CC(COC(N)=O) (CCC)COC(N)=O,x
metoprolol root root COCCC1=CC=C(OCC(O)CNC(C)C)C=C1,x
mianserin root root CN1CCN3C(C2=C(CC4=CC=CC=C34)C=CC=C2)C1,x
moprolol root root COC(C=CC=C1)=C1OCC(CNC(C)C)O,x
myrtan root root CC1CCC(C2)C(C) (C)C21,x
myrten root root CC1=CCC(C2)C(C) (C)C21,x
nicainoprol root root CC(NCC(COC1=CC=CC2=C1N(C(C3=CC=CN=C3)=O)CCC2)O)C,x
nitrogendioxide root root O,x,=,x, [N+], 16@x, [O-], x
nitricoxide root root N, 32@x, =O,x
nitrousoxide root root N#[N+] [O-], x
ozone|trioxygen root root O=[O+] [O-], x
oxaceprol root root CC(N1CC(CC1C(O)=O)O)=O,x
pelanserlin root root O=C2NC1=CC=CC=C1C(N2CCCN3CCN(C4=CC=CC=C4)CC3)=O,x
phencyclone root root O=c(c(c5c3c4cccc4c6cccc56)c2cccc2)c3c1cccc1,x
phenindione root root O=C(C2=C1C=CC=C2)C(C3=CC=CC=C3)C1=O,x
propranolol root root OC(CNC(C)C)COC1cccc2cccc12,x
psoralen root root
o,1, Ring, Ring1, c,2, (=O), x,c,3,c,4,c,x, Ring, Ring2, c,5,c,x, Ring, Ring3, c,4', c,5', o,
x,c,x, Ring, Ring3, c,8|8', c,x, Ring, Ring2, Ring, Ring1
thioct root root CCCCC1SSCC1,x
phosphoramidate|phosphorustriamide root root P(=O), x, (,x,N,n,) (,x,N,n',), x,N,n''
pyrophosphoramidate|diphosphoramidate root root
P(=O), x, (,x,N,n,) (,x,N,n',), x,O,x,P(=O), x, (,x,N,n',), x,N,n''
prolintane root root CCCC(N2CCCC2)CC1=CC=CC=C1,x
resorufin root root
c,7, Ring, Ring1, c,6,c,5a, Ring, Ring2, o,5,c,4a, Ring, Ring3, c,4,c,3, (=O), x,c,2,c,1,c,
10a, Ring, Ring3, n,10,c,9a, Ring, Ring2, c,9,c,8, Ring, Ring1
retin root root
C,15,C,14,=,x,C,13, (,x,C,20,), x,C,12,=,x,C,11,C,10,=,x,C,9, (,x,C,19,), x,C,8,=,x,
C,7,C,6, Ring, Ring1, =,x,C,5, (,x,C,18,), x,C,4,C,3,C,2,C,1, (,x,C,16,) (,x,C,17,), x,R
ing, Ring1
ritanserlin root root
CC(N=C1SC=CN12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
seganserlin root root
CC(NC1=CC=CC=[N]12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
vinylsulfurol root root C=CC1=C(C)N=CS1,x
teoprolol root root
CC(NCC(COC3=CC=CC4=C3C=C(C)N4)O)CCN1C=NC(N(C(N2C)=O)C)=C1C2=O,x
terbuprol root root COCC(COC(C) (C)C)O,x
thyropropion aminoacid ine
C,x,c,a|alpha,C,b|beta,C,1, Ring, Ring2, =,x,c,2|ortho,C,3|m|meta,=,x,c,4, (,x,o,x,c,
,1', Ring, Ring3, =,x,c,2', c,3', =,x,c,4', (,x,o,x,), x,c,5', =,x,c,6', Ring, Ring3,) x,c,
,5,=,x,c,6, Ring, Ring2
thyroacet aminoacid ine
C,x,c,a|alpha,C,1, Ring, Ring2, =,x,c,2|ortho,C,3|m|meta,=,x,c,4, (,x,o,x,c,1', Ring,
Ring3, =,x,c,2', c,3', =,x,c,4', (,x,o,x,), x,c,5', =,x,c,6', Ring, Ring3,) x,c,5,=,x,c,
6, Ring, Ring2
toliprolol root root CC(NCC(COC1=CC=CC(C)=C1)O)C,x
tolysin root root O=C(C1=C3C(C=CC(C)=C3)=NC(C2=CC=CC=C2)=C1)OCC,x
tomoxiprole root root COC1=CC=C(C4=NC2=C(N4C(C)C)C=CC3=CC=CC=C23)C=C1,x
tricyclene|tricyclen root root CC12C(C2C3)CC3C1(C)C,x
triprolidine root root CC1=CC=C(C(C3=NC=CC=C3)=CCN2CCCC2)C=C1,x
tranexam root root C[C@H]1CC[C@H](CN)CC1,x
tropicamide root root OCC(C(N(CC)CC2=CC=NC=C2)=O)C1=CC=CC=C1,x
zipeprol root root COC(C3=CC=CC=C3)CN1CCN(CC(C(C2=CC=CC=C2)OC)O)CC1,x

thioindigo root root O=C1C4=C(C=CC=C4)SC1=C2SC(C=CC=C3)=C3C2=O,x
theophyllol root root O=C1C2=C(NC=N2)N(C)C(N1C)=O.O=C([O-])C.[Na+],x
synephrine root root OC1=CC=C(C(O)CNC)C=C1,x
sulfathiazole root root NC1=CC=C(S(NC2=NC=CS2)(=O)=O)C=C1,x
sulfadiazine root root
O=S(N,x,c,2, Ring, Ring1, n, 3, c, 4, c, 5, c, 6, n, 1, Ring, Ring1,) (C2=CC=C(N)C=C2)=O,x
strychnine root root O=C(C5)N(C4C2(CC7)C(N7C6)CC3C6=CCOC5C34)C1=C2C=CC=C1,x
squalane root root CC(CCCCC(C)CCCC(C)CCCC(C)C)CCCC(C)CCCC(C)C,x
squalene root root CC(C)=CCC\C(C)=C\C\C\C(C)=C\C\C\C=C(C)\CC/C=C(CCC=C(C)C)/C,x
spermine|neuridine|musculamine|gerontine root root NCCCNCCCCNCCCN,x
spermidine root root NCCCNCCCCN,x
scopolamine root root CN1C2CC(OC(C(CO)c4cccc4)=O)CC1C3C2O3,x
genoscolamine root root C[N+]([O-])1C2CC(OC(C(CO)C4=CC=CC=C4)=O)CC1C3C2O3,x
sendachromeal root root O=C(C(C(O)=O)=C2)C=CC2=C(C)C1=CC(C(O)=O)=C(O)C=C1,x
sorb root root C,1,C,2,=,x,C,3,C,4,=,x,C,5,C,6
quercitin root root OC1=CC(C(O3)=C(O)C(C2=C3C=C(O)C=C2O)=O)=CC=C1O,x
pulegone root root CC1CC(=O)C(=C(C)C)CC1,x
benzindopyrine|benzindopyrin root root c(CC2ccncc2)(cn3Cc4cccc4)c1c3cccc1,x
benziodarone|benziodaron root root O=C(c3cc(I)c(O)c(I)c3)c2c1cccc1oc2CC,x
benzopyrronium root root C[N+](CCC(OC(C(c2cccc2)(c3cccc3)O)=O)C1)C,x
benzothiozane|benzothiozan root root O=C(C)Nc1ccc(C=NNC(N)=S)cc1,x
benzpiperylone|benzpiperylon root root
O=C1C(Cc3cccc3)=C(c4cccc4)NN1C2CCN(C)CC2,x
benzpyrinium root root CN(C(OC1c[n+](Cc2cccc2)ccc1)=O)C,x
benzquinamide|benzquinamid root root
CCN(C(C3CN2CCc1c(C2CC3OC(C)=O)cc(OC)c(OC)c1)=O)CC,x
benzthiazide|benzthiazid root root
O=S2(c1cc(S(N)(=O)=O)c(C1)cc1N=C(CSCc3cccc3)N2)=O,x
benzthiazuron root root O=C(NC)Nc2sc1cccc1n2,x
methabenzthiazuron root root O=C(NC)N(C)c2sc1cccc1n2,x
benzvalene|benzvalen root root C13C=CC2C1C23,x
abscis|absciss root root
C,1,C,2,=,x,C,3,(C),x,C,4,=,x,C,5,C,6,(C(C)(C1)C)(C(C)=CC1=O)O,x
mobenzoxamine|mobenzoxamin root root
COc1ccc(C(c4cccc4)OCCN3CCN(CC3)CCCC(c2ccc(F)cc2)=O)cc1,x
quinuclidine|quinuclidin root root
N,1, Ring, Ring1, Ring, Ring2, C,2, C,3, C,4, (,x,C,5,C,6, Ring, Ring1,),x,C,7,C,8, Ring, Ring2
urarine root root O=C3C=CC2=C(C4=CC=CC=C4C([O-])=O)C1=CC=C([O-])C=C1CC2=C3.[Na+].[Na+],x
thorin root root OC1=C(N=NC3=C([As](O)(O)=O)C=CC=C3)C2=C(C=C(S([O-])=O)=O)C=C2)C=C1S([O-])=O.[Na+].[Na+],x
furaneol root root CC1OC(C)=C(O)C1=O,x
bicine|bicin root root O=C(O)CN(CCO)CCO,x
indanthrone root root
O=C(C3=C2C=CC=C3)C1=C(NC4=CC=C(C6=O)C(C(C7=CC=CC=C67)=O)=C4N5)C5=CC=C1C2=O,x
methone|dimedone root root
C,1,(=O),x, Ring, Ring1, C,2, C,3, (=O),x,C,4,C,5,(C)(C),x,C,6, Ring, Ring1
acrinol root root NC1=C(C=C(OC)C=C3)C3=NC2=C1C=CC(N)=C2.CC(O)C(O)=O,x
danthron root root O=C(C2=C1C=CC=C2O)C(C(O)=CC=C3)=C3C1=O,x
caffeine|cafein root root O=C(N(C)C2=C1N(C)C=N2)N(C)C1=O,x
betahistine root root CNCCC1NCCCC1,x
pyranine root root [O-]S(C(C=C4O)=C1C=CC2=C(S([O-])=O)=O)C=C(S([O-])=O)=O)C3=CC=C4C1=C23)(=O)=O.[Na+].[Na+].[Na+],x
abiet root root C,x,[C@],a-
r,2(C)C1[C@@]([C@@](CCc(C(C)C)c3)([H])C3=CC1)(C,x,C,a-t,C,a-b,2)C,x

betulin loveracid root
C[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@H](O)CC[C@]1(C)[C@@]2([H])CCC3[C@@]4([H])[C@H](C(C)=C)CC5,x
betulin root root
OC[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@H](O)CC[C@]1(C)[C@@]2([H])CC3[C@@]4([H])[C@H](C(C)=C)CC5,x
caluros root root CC(C)(c1ccccc1)CC=C(C)C,x
thymine|thymine|uracil|orot|isoorot|cytosine|isocytosine|guanine|xanthine|hypoxanthine pseudosugar unknown x,x
thymine|thymine root root
N,1, Ring, Ring1, C, 2, (=O), x, N, 3, C, 4, (=O), x, c, 5, (C), x, c, 6, Ring, Ring1
uracil root root N,1, Ring, Ring1, C, 2, (=O), x, N, 3, C, 4, (=O), x, c, 5, c, 6, Ring, Ring1
orot root root C, x, c, 6, Ring, Ring1, N, 1, C, 2, (=O), x, N, 3, C, 4, (=O), x, c, 5, Ring, Ring1
isoorot root root
C, x, c, 5, Ring, Ring1, c, 6, n, 1, c, 2, (=O), x, n, 3, c, 4, (=O), x, Ring, Ring1
cytosine root root
n, 1|prefhydro, Ring, Ring1, c, 2, (=O), x, n, 3, c, 4, (N), n, c, 5, c, 6, Ring, Ring1
isocytosine root root
n, 1|prefhydro, Ring, Ring1, c, 2, (N), x, n, 3, c, 4, (=O), n, c, 5, c, 6, Ring, Ring1
guanine pseudosugar unknown x,x
guanine root root
n, 7|prefhydro, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, c, 2, (N), n, N, 1, c, 6, (=O), x, c, 5, Ring, Ring1, Ring, Ring2
xanthine root root
n, 7|prefhydro, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, c, 2, (=O), x, n, 1, c, 6, (=O), x, c, 5, Ring, Ring1, Ring, Ring2
hypoxanthine root root
n, 7|prefhydro, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, c, 2, n, 1, c, 6, (O), x, c, 5, Ring, Ring1, Ring, Ring2
theophylline|theophylline|aminophylline|aminophyllin root root
n, 7, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, (C), x, c, 2, (=O), x, n, 1, (C), x, c, 6, (=O), x, c, 5, Ring, Ring1, Ring, Ring2
theobromine|theobromine root root
n, 7, Ring, Ring1, (C), x, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, (C), x, c, 2, (=O), x, n, 1, c, 6, (=O), x, c, 5, Ring, Ring1, Ring, Ring2
xanthopterin root root Oc1nc(N)nc2c1nc(O)cn2,x
isoxanthopterin root root O=C1C(N=CC2=O)=C(N2)NC(N)=N1,x
xanthopterid root root
n, 1, Ring, Ring1, c, 2, (N), x, n, 3, c, 4, (O), x, c, 4a, Ring, Ring2, n, 5, c, 6, (O), x, c, 7, n, 8, c, 8a, Ring, Ring1, Ring, Ring2
pterine|pterine root root
n, 1, Ring, Ring1, c, 2, (N), x, N, 3, C, 4, (=O), x, c, 4a, Ring, Ring2, n, 5, c, 6, c, 7, n, 8, c, 8a, Ring, Ring2, Ring, Ring1
aminopterin root root
O,1@x,C(CCC(C(O)=O)NC(C3=CC=C(C=C3)NCC1=CN=C2C(C(N)=NC(N)=N2)=N1)=O)=O,x
vitaminh root root O=C(N2)NC1C2CS[C@H]1CCCC(O)=O,x
brucine root root
O=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCOC5[C@]34[H])C1=C2C=C(OC)C(OC)=C1,x
struchnine root root
O=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCOC5[C@]34[H])C1=C2C=,x,C,10,C,11,=C1,x
penicillan root root
C, x, [C@H], 3, Ring, Ring2, N, 4, Ring, Ring1, C, 5, (, x, [C@H], 6, ([H]), x, [C@H], 6a, Ring, Ring1, ([H]), x, S, 1, C, 2, Ring, Ring2, (C)C)=O,x

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cephalosporan root root
C,x,C,4, Ring, Ring1, =, x, C, 3, (COC(C)=O), x, C, 2, S, 1, [C@@], 7a, (, x, [C@H], 7, Ring, Ring2,
[H], x, ) , x, ([H]), x, N, 5, Ring, Ring1, C, 6, Ring, Ring2, =O, x
vitaminb1|thiamine|thiamin|thiaminechloride|thiaminchlorid root root
O3.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[Cl-], x
vitaminb1nitrate|thiaminenitrate|thiaminnitrate root root
O3.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[O-][N+]( [O-])=O, x
thiaminedisulfide root root
CC(N(C=O)CC1=CN=C(N=C1N)C)=C(SSC(CCO)=C(N(C=O)CC2=C(N)N=C(C)N=C2)C)CCO, x
vitaminb2|riboflavin root root
CC1=CC2=C(N=C(C(N3)=O)C(N2C[C@@H](O)[C@@H](O)[C@@H](O), x, C, 5', O)=NC3=O)C=C1C, x
vitamine|alphatocopherol|atocopherol root root
CC1=C2C(O[C@@](CCC[C@H](C)CCC[C@H](C)C)(C)CC2)=C(C)C(C)=C1O, x
phenolsulfonphthalein|phenolsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (, x, O, x, ) , x, c, 5', c, 6', Ri
ng, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', c, 3'', c, 4'', (, x, O, x, ) , x, c, 5'', c, 6'', Ring, Rin
g4
m cresolsulfonphthalein|m cresolsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', (O), x, c, 3', c, 4', (, x, C, x, ) , x, c, 5', c
, 6', Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', (O), x, c, 3'', c, 4'', (, x, C, x, ) , x, c, 5'', c,
6'', Ring, Ring4
o cresolsulfonphthalein|o cresolsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (, x, C, x, ) , x, c, 5', c
, 6', Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', c, 3'', (O), x, c, 4'', (, x, C, x, ) , x, c, 5'', c,
6'', Ring, Ring4
pyrocatecholsulfonphthalein|pyrocatecholsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (, x, O, x, ) , x, c, 5', c
, 6', Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', c, 3'', (O), x, c, 4'', (, x, O, x, ) , x, c, 5'', c,
6'', Ring, Ring4
pyrogallolsulfonphthalein|pyrogallolsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', (, x, O, x, ) , x, c, 3', (O), x, c, 4', (, x, O,
x, ) , x, c, 5', c, 6', Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', (, x, O, x, ) , x, c, 3'', (O), x, c,
4'', (, x, O, x, ) , x, c, 5'', c, 6'', Ring, Ring4
thymolsulfonphthalein|thymolsulfonephthalein root root
C,1, Ring, Ring1, (, x, O, 2, S, 3, (=O) (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring,
Ring2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', (, x, C(C)C, x, ) , x, c, 3', c, 4', (, x, O, x,
) , x, c, 5', (C), x, c, 6', Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', (, x, C(C)C, x, ) , x, c, 3'',
c, 4'', (, x, O, x, ) , x, c, 5'', (C), x, c, 6'', Ring, Ring4
phenolphthalein root root
C,1, Ring, Ring1, (, x, O, 2, C, 3, (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring
2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (, x, O, x, ) , x, c, 5', c, 6', Ring, R
ing3, ) , x, c, 1'', Ring, Ring4, c, 2'', c, 3'', c, 4'', (, x, O, x, ) , x, c, 5'', c, 6'', Ring, Ring4
m cresolphthalein root root
C,1, Ring, Ring1, (, x, O, 2, C, 3, (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring
2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', (O), x, c, 3', c, 4', (, x, C, x, ) , x, c, 5', c, 6',
Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', (O), x, c, 3'', c, 4'', (, x, C, x, ) , x, c, 5'', c, 6'',
Ring, Ring4
o cresolphthalein root root
C,1, Ring, Ring1, (, x, O, 2, C, 3, (=O), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring
2, Ring, Ring1, ) , x, (, x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (, x, C, x, ) , x, c, 5', c, 6',
Ring, Ring3, ) , x, c, 1'', Ring, Ring4, c, 2'', c, 3'', (O), x, c, 4'', (, x, C, x, ) , x, c, 5'', c, 6'',
Ring, Ring4

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pyrocatecholphthalein root root
C,1, Ring, Ring1, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x, (,x,c,1', Ring, Ring3, c,2', c,3', (O),x,c,4', (,x,O,x,) ,x,c,5', c,6', Ring, Ring3,) ,x,c,1'', Ring, Ring4, c,2'', c,3'', (O),x,c,4'', (,x,O,x,) ,x,c,5'', c,6'', Ring, Ring4
pyrogallolphthalein root root
C,1, Ring, Ring1, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x, (,x,c,1', Ring, Ring3, c,2', (,x,O,x,) ,x,c,3', (O),x,c,4', (,x,O,x,) ,x,c,5', c,6', Ring, Ring3,) ,x,c,1'', Ring, Ring4, c,2'', (,x,O,x,) ,x,c,3'', (O),x,c,4'', (,x,O,x,) ,x,c,5'', c,6'', Ring, Ring4
thymolphthalein root root
C,1, Ring, Ring1, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x, (,x,c,1', Ring, Ring3, c,2', (,x,O,x,) ,x,c,3', c,4', (,x,O,x,) ,x,c,5', (C),x,c,6', Ring, Ring3,) ,x,c,1'', Ring, Ring4, c,2'', (,x,O,x,) ,x,c,3'', c,4'', (,x,O,x,) ,x,c,5'', (C),x,c,6'', Ring, Ring4
tetraiodophthalein|iodophthalein|iodophene|iodotetragnost root root
C,1, Ring, Ring1, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4, (I),x,c,5, (I),x,c,6, (I),x,c,7, (I),x,c,7a, Ring, Ring2, Ring, Ring1,) ,x, (,x,c,1', Ring, Ring3, c,2', c,3', c,4', (,x,O,x,) ,x,c,5', c,6', Ring, Ring3,) ,x,c,1'', Ring, Ring4, c,2'', c,3'', c,4'', (,x,O,x,) ,x,c,5'', c,6'', Ring, Ring4
fluorescein root root
C,1, Ring, Ring1, Ring, Ring5, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x,c,10a, Ring, Ring3, c,1', c,2', c,3', (,x,O,x,) ,x,c,4', c,4a', Ring, Ring3, O,x,c,5b', Ring, Ring4, c,5', c,6', (,x,O,x,) ,x,c,7', c,8', c,8a', Ring, Ring5, Ring, Ring4
sulfonfluorescein root root
C,1, Ring, Ring1, Ring, Ring5, (,x,O,2,S,3,(=O)(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x,c,10a, Ring, Ring3, c,1', c,2', c,3', (,x,O,x,) ,x,c,4', c,4a', Ring, Ring3, O,x,c,5b', Ring, Ring4, c,5', c,6', (,x,O,x,) ,x,c,7', c,8', c,8a', Ring, Ring5, Ring, Ring4
fluoran|fluorane root root
C,1, Ring, Ring1, Ring, Ring5, (,x,O,2,C,3,(=O),x,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x,c,10a, Ring, Ring3, c,1', c,2', c,3', c,4', c,4a', Ring, Ring3, O,x,c,5b', Ring, Ring4, c,5', c,6', c,7', c,8', c,8a', Ring, Ring5, Ring, Ring4
uramil root root N,n,C1C(=O)NC(=O)NC(=O)1,x
isosorbide root root
O,x, [C@H],2, Ring, Ring1, C,1,O,x, [C@@],4, Ring, Ring2, (,x, [H],x,) ,x, [C@],3, Ring, Ring1, (,x, [H],x,) ,x,O,x,C,6, [C@H],5, Ring, Ring2,O,x
isoproterenol|isoprenaline root root CC(NCC(C1=CC(O)=C(O)C=C1)O)C,x
shikonin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
alkannin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
shikalkin root root CC(C)=CCC(O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
hyoscyamine root root CN1C2CCC1C[C@H](OC(C(CO)c3cccc3)=O)C2,x
44'carbocyanine|cryptocyanine|kryptocyanine root root
[n+],1, Ring, Ring1, c,2,c,3,c,4, (,x,c,4a, Ring, Ring2, c,5,c,6,c,7,c,8,c,8a, Ring, Ring2, Ring, Ring1,) ,x,C=CC=,x,C,4', Ring, Ring3, C,3', =,x,C,2', N,1', c,8a', Ring, Ring4, c,8', c,7', c,6', c,5', c,4a', Ring, Ring4, Ring, Ring3
22'carbocyanine|pinacyanol root root
[n+],1, Ring, Ring1, c,2, (,x,c,3,c,4,c,4a, Ring, Ring2, c,5,c,6,c,7,c,8,c,8a, Ring, Ring2, Ring, Ring1,) ,x,C=CC=,x,C,2', (,x,C,3', =,x,C,4', Ring, Ring3,) ,x,N,1', c,8a', Ring, Ring4, c,8', c,7', c,6', c,5', c,4a', Ring, Ring4, Ring, Ring3
oxacarbocyanine root root
o,1, Ring, Ring1, c,2, (,x, [n+],3,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ring, Ring1,) ,x,C,8, =,x,C,9,C,10, =,x,C,2', Ring, Ring3, N,3', c,3a', Ring, Ring4, c,4', c,5', c,6', c,7', c,7a', Ring, Ring4, O,1', Ring, Ring3
oxadicalcarbocyanine root root
o,1, Ring, Ring1, c,2, (,x, [n+],3,c,3a, Ring, Ring2, c,4,c,5,c,6,c,7,c,7a, Ring, Ring2, Ri

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ng,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
oxatricarbocyanine root root
o,1,Ring,Ring1,c,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
thiacyanine root root
s,1,Ring,Ring1,c,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1, ),x,C,8,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c
,7a',Ring,Ring4,S,1',Ring,Ring3
thiacarbocyanine root root
s,1,Ring,Ring1,c,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiadicarbocyanine root root
s,1,Ring,Ring1,c,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiatricarbocyanine root root
s,1,Ring,Ring1,c,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
selenacarbocyanine root root
[se],1,Ring,Ring1,cC,2, (,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1, ),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4'
,c,5',c,6',c,7',c,7a',Ring,Ring4,[Se],1',Ring,Ring3
hordenine root root CN(C)CCC1=CC=C(O)C=C1,x
maltol root root o1ccc(=O)c(O)c(C)1,x
coman root root Cc1=cc(=O)ccO1,x
chrysoidine root root
c,4|p|para, (,x,c,3|m|meta,c,2|o|ortho,Ring,Ring1, ),x,c,5,c,6,c,1,Ring,Ring1,N=Nc
2c(N)cc(N)cc2,x
alphafuril root root O=C(C1=CC=CO1)C(C2=CC=CO2)=O,x
anisil root root O=C(C1=CC=C(OC)C=C1)C(C2=CC=C(OC)C=C2)=O,x
alphaphellandrene root root CC1=CCC(C(C)C)C=C1,x
betaphellandrene root root CC(C(C=C1)CCC1=C)C,x
scopolamine|scopolamin root root C[N+](O-
)C2CCC1CC(OC(C(CO)C3=CC=CC=C3)=O)C2,x
pilocarpine|pilocarpin root root CC[C@H]1[C@@H](CC2=CN=CN2C)COC1=O,x
guanethidine root root NC(NCCN1CCCCC1)=N,x
lobeline root root CN1C(CC(C3=CC=CC=C3)O)CCCC1CC(C2=CC=CC=C2)=O,x
mercaptur root root C[C@H](CS)NC(C)=O,x
phenylmercaptur root root C[C@H](CS1CCCCC1)NC(C)=O,x
alpalip|alip root root CCCCC1SSCC1,x
perill|perilla root root CC1=CCC(C(C)=C)CC1,x
biotin root root O,1@x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
biotinyl root root C,4@x,{CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
biotinamide|biotinamid root root
N,x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
bisphenola root root
O1.Oc,4,Ring,Ring2,c,5,c,6,c,1, (,x,c,2,c,3,Ring,Ring2, ),x,C(C)(C),x,c,1',Ring,Ri
ng3,c,2',c,3',c,4',Ring,Ring1,c,5',c,6',Ring,Ring3
pantothen root root CCCNC(C(C(CO)(C)C)O)=O,x
alloxan root root
N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,C,5,(=O),x,C,6,(=O),x,Ring,Ring1
croman root root Cc1occc(=O)c1,x

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cinchon root root
C,9,(,x,c,4',Ring, Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring, Ring4,),(,x,c,8a',Ring,
Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
t,Ring, Ring2,),(,x,c,8,Ring, Ring1,N(CC3)CC(,x,c,10,=,x,c,11,)C3C1,x
1011dihydrocinchon root root
C,9,(,x,c,4',Ring, Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring, Ring4,),(,x,c,8a',Ring,
Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
t,Ring, Ring2,),(,x,c,8,Ring, Ring1,N(CC3)CC(,x,c,10,c,11,)C3C1,x
cinchonine|cinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
1011dihydrocinchonine|1011dihydrocinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
quinidine root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroquinidine root root
O[C@@H]([C@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
cinchonidine|cinchonidin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
1011dihydrocinchonidine|1011dihydrocinchonidin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
quinine|quinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
ydroquinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
hepes root root S,x,(=,x,O,x,),(,x,=O,x,),(,x,O,1@o,),(,x,CCN(CC1)CCN1CCO,x
pipes root root O=S(CCN1CCN(CCS(=O)(O)=O)CC1)(O)=O,x
popop root root C1(C2=CC=C(C4=NC=C(C5=CC=CC=C5)O4)C=C2)=NC=C(C3=CC=CC=C3)O1,x
dibenzosuber root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,4a,Ring, Ring2,c,5,c,5a,Ring, Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring, Ring3,c,10,c,11,c,11a,Ring, Ring2,Ring, Ring1
benzosuber root root
c,1,Ring, Ring1,c,2,c,3,c,4,c,5,c,5a,Ring, Ring2,c,6,c,7,c,8,c,9,c,9a,Ring, Ring2,R
ing, Ring1
orthosilicate root root
[Si],x,(,x,O,1@o''',),x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
orthotitanate root root
[Ti],x,(,x,O,1@o''',),x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
gona|gon root steroid
C,3,(,x,c,2,c,1,Ring, Ring1,),(,x,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14,Ri
ng, Ring4,c,15,c,16,c,17,c,13,Ring, Ring4,c,12,c,11,c,9,Ring, Ring3,c,10,Ring, Ring1
,Ring, Ring2
estra|oestra|estr|oestr root steroid
C,3,(,x,c,2,c,1,Ring, Ring1,),(,x,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14,Ri
ng, Ring4,c,15,c,16,c,17,[C@@],13,Ring, Ring4,(,x,c,x,),(,x,c,12,c,11,c,9,Ring, Ring3
,c,10,Ring, Ring1,Ring, Ring2
equilen root steroid
c,3,(O)(,x,c,2,c,1,Ring, Ring1,),(,x,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14
,Ring, Ring4,c,15,c,16,c,17,(=O),x,[C@@],13,Ring, Ring4,(,x,c,x,),(,x,c,12,c,11,c,9,
Ring, Ring3,c,10,Ring, Ring1,Ring, Ring2
dihydroequilen root steroid
c,3,(O)(,x,c,2,c,1,Ring, Ring1,),(,x,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14
,Ring, Ring4,c,15,c,16,c,17,(O),x,[C@@],13,Ring, Ring4,(,x,c,x,),(,x,c,12,c,11,c,9,
Ring, Ring3,c,10,Ring, Ring1,Ring, Ring2
androsta|androst|etiochola|etiochol root steroid
C,3,(,x,c,2,c,1,Ring, Ring1,),(,x,c,4,c,5,Ring, Ring2,c,6,c,7,c,8,Ring, Ring3,c,14,Ri

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ng, Ring4, C, 15, C, 16, C, 17, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
etioallochola|etioallochol root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, [C@@], 5, ([H]), x, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, C, 17, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
etien root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, =, x, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (C), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
etian root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (C), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
androstenediol root steroid
[C@H], 3, (O), x, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, =, x, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@H], 17, (O), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
androstenedione root steroid
C, 3, (=O), x, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, =, x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, C, 17, (=O), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
pregna|pregn root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, C, 20, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
allopregna|allopregn root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, [C@@], 5, ([H]), x, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, C, 20, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
chola|chol root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
cholesta|cholest|coprost root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
lanosta|lanost root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, [C@], 4, (, x, C, 28,) (, x, C, 29,), x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, [C@], 14, Ring, Ring4, (, x, C, 30,), x, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
dammara|dammar root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, [C@], 4, (, x, C, 28,) (, x, C, 29,), x, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, [C@@], 14, Ring, Ring4, (, x, C, 30,), x, C, 15, C, 16, [C@], 17, (, x, [C@@], 20, (, x, C, 22, C, 23, C, 24, C, 25, (, x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
urs root steroid
C, 3, (, x, C, 2, C, 1, Ring, Ring1,), x, C, 4, (, x, C, x,) (, x, C, x,), x, C, 5, Ring, Ring2, C, 6, C, 7, [C@], 8, (C), x, Ring, Ring3, [C@], 14, Ring, Ring4, (C), 27, C, x, C, x, [C@@], x, Ring, Ring5, (C), 28, C, 22, C, 21, [C@@H], 20, (, x, C, 30,), x, [C@H], 19, (, x, C, 29,), x, [C@@], 18, ([H]), x, Ring, Ring5, [C@@], 13, Ring, Ring4, (, x, [H], x,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, x

,20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
ergosta|ergost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
campesta|campest root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
poriferasta|poriferast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(CC),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
stigmasta|stigmast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(,x,C,28,C,29,)),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
pregnenolone root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
prednisolone|prednisolon root steroid
C,1,Ring,Ring1,=,x,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,(,x,O,x,),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
progesterone|progesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
tetrahydroprogesterone|tetrahydroprogesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
hydrocortisone|hydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dihydrocortisone|dihydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
tetrahydrocortisone|tetrahydrocortison root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
cortisone|cortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13

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,Ring,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring
1,Ring,Ring2,C,19
androsterone root steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9
,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
isoandrosterone root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,
Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,
Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
aldosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,1
8,=O,x,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,1
9
pregnanolone root steroid
C,3,(O)(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C
,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
testosteron|testosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dihydrotestosteron|dihydrotestosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
oestradiol|estradiol|betaoestradiol|betaestradiol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11
,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestriol|estriol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,[C@@],16,(O),x,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x
,C,12,C,11,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestrone|estrone root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C
,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
brassinolid|brassinolide root steroid
[C@@H],3,(O),x,(,x,[C@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@],5,Ring,Ring2,([H]),
x,C,6,(=O)O,x,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,
(,x,[C@H],22,(O),x,[C@H],23,(O),x,[C@@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
calcdiol root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,2
5,(,x,C,26,)(O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
calciol|cholecalciferol|vitamind3 root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8|
a-
r,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C
,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11|a-
t,C,9|a-b,Ring,Ring3,,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19

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bufadienolide root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,C,16, [C@],17,(,x,[C@@],20, Ring, Ring5,=,x,C,21,O,x,C,24,(=O),x,C,23,=,x,C,22, Ring, Ring5,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

cev root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,[C@@],14,([H]),x, Ring, Ring4,C,15,C,16,[C@@],17,([H]),x, Ring, Ring5,[C@@H],20,(C),x,[C@@],x,([H]),x, Ring, Ring6,C,x,C,x,[C@H],x,(C),x,C,x,N,x, Ring, Ring6,C,x,[C@],x,([H]),x, Ring, Ring5,[C@@],12,([H]),x, Ring, Ring4,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

solidan root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,C,16, Ring, Ring5,[C@],17,([H])(,x,[C@],20,(,x,C,21,) ,x,[C@],22,([H]),x, Ring, Ring6,C,23,C,24,[C@H],25,(,x,C,27,) ,x,C,26,N,28, Ring, Ring6, Ring, Ring5,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

spirost root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,[C@],16,([H])(,x,O,x, Ring, Ring5,) ,x,[C@],17,([H])(,x,[C@@],20,(,x,[C@@],22, Ring, Ring5,(,x,O,x, Ring, Ring6,) ,x,C,23,C,24,C,25,(,x,C,26, Ring, Ring6,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

spirosol root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,[C@],16,([H])(,x,O,x, Ring, Ring5,) ,x,[C@],17,([H])(,x,[C@],20,(,x,C,22, Ring, Ring5,(,x,N,x, Ring, Ring6,) ,x,C,23,C,24,C,25,(,x,C,26, Ring, Ring6,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

tomatid root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,[C@@H],5,([H]),x, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,[C@],16,([H])(,x,O,x, Ring, Ring5,) ,x,[C@],17,([H])(,x,[C@],20,(,x,[C@],22, Ring, Ring5,(,x,N,x, Ring, Ring6,) ,x,C,23,C,24,[C@@H],25,(,x,C,26, Ring, Ring6,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

solasod root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,[C@@H],5,([H]),x, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,[C@],16,([H])(,x,O,x, Ring, Ring5,) ,x,[C@],17,([H])(,x,[C@],20,(,x,[C@@],22, Ring, Ring5,(,x,N,x, Ring, Ring6,) ,x,C,23,C,24,[C@H],25,(,x,C,26, Ring, Ring6,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

furost root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,[C@],16,([H])(,x,O,x, Ring, Ring5,) ,x,[C@],17,([H])(,x,[C@@],20,(,x,[C@],22, Ring, Ring5,C,23,C,24,C,25,(,x,C,26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

chol loveracid steroid

C,1, Ring, Ring1,C,2,[C@H],3,(O),x,C,4,C,5, Ring, Ring2,C,6,[C@@H],7,(O),x,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,[C@@H],12,(O),x,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

lithochol loveracid steroid

C,1, Ring, Ring1,C,2,[C@@H],3,(O),x,C,4,C,5, Ring, Ring2,C,6,C,7,C,8, Ring, Ring3,C,14, Ring, Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4,(,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3,[C@@],10, Ring, Ring1, Ring, Ring2,C,19

tetrachloroiodate|iodotetrachloride root root [I-](Cl)(Cl)(Cl)Cl,x
chlorochromate root root [O-][Cr](=O)(=O)Cl,x
fluorochromate root root [O-][Cr](=O)(=O)F,x
fluoroborate|fluoroborat|tetrafluoroborate|tetrafluoroboratel|tetrafluoroborat|b
f4|borofluoride|borofluorid|fluoborate|fluoborat root root [B-](F)(F)(F)F,x
fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat root root [Si-
-](F)(F)(F)(F)(F)F,x
borohydride|borohydrid root root [B-],x
borodeuteride|borodeuterid root root [B-]([2H])([2H])([2H])[2H],x
cyanoborodeuteride|cyanoborodeuterid root root [B-]([2H])([2H])([2H])C#N,x
aluminumhydride|aluminumhydrid root root [Al-],x
persulfate|persulfat|peroxodisulfate|peroxodisulfat root root
O,1@x,S(=O)(=O)OOS(=O)(=O),x,O,1@x
bifluoride|bifluorid root root [F-],x,[H]F,x
water root root [H]O[H],x
hydrofluoride root hydrochloride [H]F,x
hydrochloride|hcl root hydrochloride [H]Cl,x
2hcl root hydrochloride [H]Cl.[H]Cl,x
3hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl,x
4hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl,x
5hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl.[H]Cl,x
methochloride|chlormethylate root hydrochloride CCl,x
methobromide|brommethylate root hydrochloride CBr,x
hydrobromide|hbr root hydrochloride [H]Br,x
2hbr root hydrochloride [H]Br.[H]Br,x
3hbr root hydrochloride [H]Br.[H]Br.[H]Br,x
4hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br,x
5hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br.[H]Br,x
hydrotribromide|hbr root hydrochloride [H]Br(Br)Br,x
hydroiodide|hydriodide root hydrochloride [H]I,x
methoiodide|methiodide root hydrochloride CI,x
ethoiodide|ethiodide root hydrochloride CCI,x
hydrate|h2o root hydrochloride [H]O[H],x
deuterate|d2o root hydrochloride [2H]O[2H],x
etherate root hydrochloride
O(C([H])([H])C([H])([H])([H])C([H])([H])C([H])([H])([H])x
bitartrate|bitartrate|hydrogentartrate root hydrochloride
O,1@x,C,1,(=,x,O,x),x,C,2,(=,x,O,x),x,C,3,(=,x,O,x),x,C,4,(=,x,O),x,O,x,[H],x
dbitartrate|hydrogendtartrate root hydrochloride
O,1@x,C,1,(=,x,O,x),x,[C@H],2,(=,x,O,x),x,[C@H],3,(=,x,O,x),x,C,4,(=,x,O),x,O,
x,[H],x
lbitartrate|hydrogenltartrate root hydrochloride
O,1@x,C,1,(=,x,O,x),x,[C@H],2,(=,x,O,x),x,[C@H],3,(=,x,O,x),x,C,4,(=,x,O),x,O,
x,[H],x
bimaleate|hydrogenmaleate root hydrochloride
O,1@x,C,1,(=,x,O,x),x/,x,C,2,=,x,C,3,\,x,C,4,(=,x,O),x,O,x,[H],x
bisuccinate|hydrogensuccinate root hydrochloride
O,1@x,C,1,(=,x,O,x),x,C,2,C,3,C,4,(=O)O[H],x
bipthalate root hydrochloride
O,1@x,C(=O),x,c,1, Ring, Ring1, c,2, (C(=O)O[H]),x,c,3,c,4,c,5,c,6, Ring, Ring1
hydrogenoxalate root hydrochloride
O,1@x,C,1,(=,x,O,x),x,C,2,(=,x,O),x,O,x,[H],x
bisulfate|bisulfat|hydrogensulfate root root O,1@x,S(=O)(=O)O[H],x
bisulfite|bisulfid|hydrogensulfite root root O,1@x,S(=O)O[H],x
bisulfide|bisulfid|hydrogensulfide root root S,1@x,[H],x
glycol|cellosolve|cellosolv root glycol
C,1|a|alpha, Ring, Ring1, C,2|b|beta, O,1@x,,x,O,1@x, Ring, Ring1

thioglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2|b|beta, S,1@x, ., x, O,1@x, Ring, Ring1
 dithioglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2 b|beta, S,1@x, ., x, S,1@x, Ring, Ring1
 selenoglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2|b|beta, [Se],1@x, ., x, O,1@x, Ring, Ring1
 diselenoglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2|b|beta, [Se],1@x, ., x, [Se],1@x, Ring, Ring1
 telluroglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2|b|beta, [Te],1@x, ., x, O,1@x, Ring, Ring1
 ditelluroglycol root glycol
 C,1|a|alpha, Ring, Ring1, C,2|b|beta, [Te],1@x, ., x, [Te],1@x, Ring, Ring1
 tempo root root
 C,4, Ring, Ring1, C,5, C,6, (C) (C), x, N,1, (, x, O,16@x,) , x, C,2, (C) (C), x, C,3, Ring, Ring1
 proxyl root root
 C,3, Ring, Ring1, C,2, (C) (C), x, N,1, (, x, O,16@x,) , x, C,5, (C) (C), x, C,4, Ring, Ring1
 nitroxide|nitroxyl root root N,n, O,16@x
 nitramine root root N,n, [N+] (=O) [O-], x
 nitramino root root N,4@n, [N+] (=O) [O-], x
 special-oxine root root
 n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, (O), x, c,8a, Ring, Ring1, Ring, Ring2
 special-azine|ketazine root azine N,8@x, N,8@x
 oxime|oxim|antioxime root oxime N,8@x, O, o
 hydrazone|hydrazon root oxime N,8@x, N, n
 semicarbazone|semicarbazon root oxime N,8@1, N,2, C,3, (=, x, O, x,) , x, N,4
 azino root bridge N,8@x, N,8@x
 azimino root bridge N,4@x, N, x, =, x, N,4@x
 biimino|biimin root bridge N,4@x, N,4@x
 epidioxy root bridge O,4@x, O,4@x
 epidithio|epidithi root bridge S,4@x, S,4@x
 epimino root bridge N,5@x
 epithio root bridge S,5@x
 episeleno root bridge [Se],5@x
 epitelluro root bridge [Te],5@x
 epithioximino|epithioximin root bridge S,4@x, O, x, N,4@x
 epoxy root bridge O,5@x
 epoxyimino|epoxyimin root bridge O,4@x, N,4@x
 epoxynitrilo root bridge O,4@x, N,8@x
 epoxythio|epoxythi root bridge O,4@x, S,4@x
 epoxythioxy root bridge O,4@x, S, x, O,4@x
 epitritio|epitriti root bridge S,4@x, S, x, S,4@x
 cyanohydrin root oxime O,4@x, ., x, C,4@x, #N, x
 fluorohydrin root oxime O,4@x, ., x, F,4@x
 chlorohydrin root oxime O,4@x, ., x, Cl,4@x
 bromohydrin root oxime O,4@x, ., x, Br,4@x
 iodohydrin root oxime O,4@x, ., x, I,4@x
 acetal|ketal|semiacetal|demiacetal|hemiactal|semiketal|demiketal|hemiketal|glyc
 olacetal|glycolketal root oxime O,4@x, ., x, O,4@x
 mercaptal|mercaptole root oxime S,4@x, ., x, S,4@x
 ketone|keton root ketone C, x, =, x, O, x
 ketoxime root ketone C, x, =, x, N, x, O, x
 ketoximino root ketone C, x, =, x, N, x, O,4@x
 ketyl root ketone C,4@x, [O-], x
 sulfoxide|sulfoxid root ketone S, x, =, x, O, x
 sulfone|sulfon root ketone S, x, (=, x, O, x,) , x, =, x, O, x
 sulfimide|sulfimid|sulfilimine|sulfilimin root ketone S, x, =, x, N, x

sulfoximide|sulfoximid|sulfoximine|sulfoximin root ketone
S,x,(=,x,O,x,),x,=,x,N,x
selenoxide|selenoxid root ketone [Se],x,=,x,O,x
selenone|selenon root ketone [Se],x,(=,x,O,x,),x,=,x,O,x
selenimide|selenimid root ketone [Se],x,=,x,N,x
selenoximide|selenoximid root ketone [Se],x,(=,x,O,x,),x,=,x,N,x
telluroxide|telluroxid root ketone [Te],x,=,x,O,x
tellurone|telluron root ketone [Te],x,(=,x,O,x,),x,=,x,O,x
tellurimide|tellurimid root ketone [Te],x,=,x,N,x
telluroximide|telluroximid root ketone [Te],x,(=,x,O,x,),x,=,x,N,x
peroxide|peroxid root ketone O,x,O,x
persulfide|persulfid root ketone S,x,S,x
formal root ketone O,x,Ring,Ring1,,x,O,x,C,x,Ring,Ring1
ether root ether O,x
etherof root ofether O,x
thioether root ether S,x
selenoether root ether [Se],x
telluroether root ether [Te],x
oin oin unknown C,1@b|beta,(O),x,C,1@a|alpha,=O,x
ano methanomaker unknown x,x
quinone|quinon suffix quinone O,8@x
quinodimethane|quinodimethan suffix quinone C,10@x
radical radical unknown x,x
yl suffix yl 1,yl
ylidene|yliden|ilidene|iliden| suffix yl 2,yl
ylidyne|ylidyn|ilidyne|ilidyn suffix yl 3,yl
ane|an suffix ignore x,x
ine|in suffix ignore x,x
ene|en suffix bondchange 2,bond
yne|yn suffix bondchange 3,bond
thiol|ylthiol suffix suffix S,4@s
ol suffix olsuffix O,4@x
olate suffix suffix [O-],4@x
anethiolate|thiolato suffix suffix [S-],4@x
one|on suffix reqcarbon O,8@x
thione suffix reqcarbon S,8@x
selenone|selone suffix reqcarbon [Se],8@x
tellurone suffix reqcarbon [Te],8@x
imine root oxime N,8@n
imine imine suffix N,8@n
iminium root oxime [N+],8@x
iminium imine suffix [N+],8@x
glycol glycol unknown O,4@o,,x,O,4@o'
thioglycol glycol unknown S,4@s,,x,O,4@o
dithioglycol glycol unknown S,4@s,,x,S,4@s'
selenoglycol glycol unknown [Se],4@x,,x,O,4@x
diselenoglycol glycol unknown [Se],4@x,,x,[Se],4@x
telluroglycol glycol unknown [Te],4@x,,x,O,4@x
ditelluroglycol glycol unknown [Te],4@x,,x,[Te],4@x
cyanohydrin glycol unknown C,4@x,#N,x,,x,O,4@x
fluorohydrin glycol unknown F,4@x,,x,O,4@x
chlorohydrin glycol unknown Cl,4@x,,x,O,4@x
bromohydrin glycol unknown Br,4@x,,x,O,4@x
iodohydrin glycol unknown I,4@x,,x,O,4@x
oxide counterion oxide O,3@x
sulfide|mercaptide counterion oxide S,8@x
selenide counterion oxide [Se],8@x

telluride counterion oxide [Te],8@x
 methanoxymethano root methanobridge C,4@x,O,x,C,4@x
 etheno root methanobridge C,4@x,=,x,C,4@x
 metheno root metheno C,5@x
 obenzeno root methanobridge c,4@x,ring,ring1,c,4@x,c,x,c,x,c,x,c,x,ring,ring1
 epoxide|enoxide counterion bridge O,5@x
 episulfide counterion bridge S,5@x
 sultam counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,N,4@x
 sultone|sultone counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,O,4@x
 dicarboximide|dicarboxylicimide|dicarboxylicacidimide counterion bridge
 C,4@x,(=,x,O,x,),x,N,x,C,4@x,=,x,O,x
 dicarboximido counterion bridge
 C,4@x,(=,x,O,x,),x,ring,ring1,.,x,C,4@x,ring,ring2,=,x,O,x,.,x,N,4@x,ring,ring1,
 ring,ring2
 carbolactam counterion bridge C,4@x,(=,x,O,x,),x,O,4@x
 nitride counterion ionable N,12@x
 phosphide counterion ionable P,12@x
 antimonide counterion ionable [Sb],12@x
 arsenide counterion ionable [As],12@x
 hydroxide|hydroxid counterion ionable O,4@x
 deuterioxide|deuteroxid counterion ionable O,4@x,[2H],x
 hydrosulfide|hydrosulfid|sulfhydrate|sulfhydrat counterion ionable S,4@x
 hydroselenide|hydroselenid counterion ionable [Se],4@x
 hydrotelluride|hydrotellurid counterion ionable [Te],4@x
 hydride|hydrid counterion ionable [H],4@1
 deuteride|deuterid counterion ionable [2H],4@1
 fluoride|fluorid counterion ionable F,4@1
 chloride|chlorid|muriate counterion ionable Cl,4@1
 bromide|bromid counterion ionable Br,4@1
 iodide|iodid counterion ionable [I],4@1
 acetylde counterion ionable C,4@x,#[C-],x
 cyanide|cyanid counterion ionable C,4@x,#N,x
 isocyanide|isocyanid|isonitrile counterion ionable [N+],4@x,#[C-],x
 cyanate|cyanat counterion ionable O,4@x,C#N,x
 isocyanate|isocyanat counterion ionable N,4@x,=C=O,x
 fulminate|fulminat counterion ionable O,4@x,[N+][C-],x
 thiocyanate|thiocyanat|sulfocyanate|sulfocyanat|sulfocyanide|sulfocyanid|rhodani
 de|rhodanid counterion ionable S,4@x,C#N,x
 isothiocyanate|isothiocyanat|isorhodanide|isorhodanid counterion ionable
 N,4@x,=C=S,x
 selenocyanate|selenocyanat counterion ionable [Se],4@x,C#N,x
 isoselenocyanate|isoselenocyanat counterion ionable N,4@x,=C=[Se],x
 tellurocyanate|tellurocyanat counterion ionable [Te],4@x,C#N,x
 isotellurocyanate|isotellurocyanat counterion ionable N,4@x,=C=[Te],x
 azide|azid counterion ionable N,4@x,[N+]=[N-],x
 sulfenamide|sulfenamid counterion counterion S,4@x,N,n
 sulfonazide counterion counterion S,4@x,(=O)(=O)N[N+][N-],x
 alcohol|icalcohol counterion counterion O,4@x
 deuterol counterion counterion O,4@x,[2H],x
 selenol counterion counterion [Se],4@s
 tellurol counterion counterion [Te],4@s
 nitrile|nitril counterion counterion N,12@x
 carbonitrile|carbonitril counterion counterion C#N,4@x
 diazonium counterion counterion [N+],4@x,#N,x
 mercaptan|thioalcohol counterion counterion S,4@x
 hydroperoxide|hydroperoxid counterion ionable O,4@x,O,x

carboxaldehyde|carboxaldehyd|carboxyaldehyde|carboxyaldehyd|carbonal counterion
counterion C,4@x,(=O),x
carboxaldoxime|carboxaldoxim counterion counterion C,4@x,(=NO),x
carbamidine counterion counterion C,4@x,(=,x,N,1@n'|n2),x,N,2@n|n1
oxyfluoride counterion bridge F,4@x,,x,O,8@x
oxychloride counterion bridge Cl,4@x,,x,O,8@x
oxybromide counterion bridge Br,4@x,,x,O,8@x
oxyiodide counterion bridge I,4@x,,x,O,8@x
thiochloride counterion bridge Cl,4@x,,x,S,8@x
oxylradical counterion counterion O,20@x
carbo|carb carbeth root C,4@x,(=O),x
dioxyl infix infix O,4@x,O,x
oxy infix doublebondable O,4@x
peroxy infix doublebondable O,4@x,O,x
sulfanyl infix infix S,4@x
thio infix doublebondable S,4@x
mercapto infix infix S,4@x
seleno infix doublebondable [Se],4@x
telluro infix doublebondable [Te],4@x
amino|amin infix infix N,4@n|w|omega
phosphino infix infix P,4@n|w|omega
phosphinyl infix infix [PH3],4@x,(=,x,O,x),x
arsino infix infix [As],4@n|w|omega
stibino infix infix [Sb],4@n|w|omega
bismuthino infix infix [Bi],4@n|w|omega
hydrazino infix infix N,2|n',N,4@1|n
hydroximino infix infix N,3@n,O,x
imino|imin infix infix N,8@n
imino|imin imine infix N,4@n
iminio infix infix [N+],8@n
iminio imine infix [N+],4@n
nitrilo infix infix N,12@n
hydrazono infix infix N,8@x,N,n
oximino infix infix N,8@x,O,o
amidosulfen infix infix S,x,N,n
sulfen infix infix S,x
sulfen infix doublebondable S,x,(=O),x
selenen infix infix [Se],x
carbonyl infix carbonyl C,4@x,(=O),x
thiocarbonyl infix carbonyl C,4@x,(=S),x
selenocarbonyl infix carbonyl C,4@x,(=[Se]),x
tellurocarbonyl infix carbonyl C,4@x,(=[Te]),x
thionyl infix carbonyl S,4@x,(=O),x
sulfuryl infix carbonyl S,4@x,(=O)(=O),x
carbonothioyl infix carbonyl C,4@x,(=S),x
carbonimidoyl infix carbonyl C,4@x,(=N),x
carbamo|carbam infix trivial C,x,(=,x,O,x),x,N,n|w|omega
nitrilomethylidyne root bridge C,4@x,=,x,N,4@x
diazo azo diazo N,4@x,=,x,N,x
azo infix doublebondable N,4@x,=,x,N,x
azo root bridge N,4@x,=,x,N,4@x
azo azo root N,x,=,x,N,x
hydrazo infix doublebondable N,x,N,4@x
hydrazo root bridge N,4@x,N,4@x
hydrazo azo root N,1@x,N,1@x
nnoazoxy|azoxy infix doublebondable [N+],4@x,([O-]),x,=,x,N,x
nnoazoxy|azoxy root bridge [N+],4@x,([O-]),x,=,x,N,4@x

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azoxy azo root [N+],x,([O-]),x,=,x,N,x
azodioxy azo root [N+],x,([O-]),x,=,x,[N+],x,[O-],x
azodioxy infix doublebondable [N+],4@x,([O-]),x,=,x,[N+],x,[O-],x
azodioxy root bridge [N+],4@x,([O-]),x,=,x,[N+],4@x,[O-],x
onnazoxy|nonazoxy infix doublebondable N,4@x,=,x,[N+],x,[O-],x
diazoamino azo root N,x,=,x,N,x,N,n
diazoamino root bridge N,4@x,=,x,N,x,N,4@n
mercuri infix infix [Hg],4@x
per prefix permult x,x
bi prefix ringmult 2,mult
ter prefix ringmult 3,mult
quater prefix ringmult 4,mult
quinque prefix ringmult 5,mult
sexi prefix ringmult 6,mult
septi prefix ringmult 7,mult
octi prefix ringmult 8,mult
novi prefix ringmult 9,mult
deci prefix ringmult 10,mult
kis prefix kis 1,x
mono|mon prefix prefix 1,mult
hen prefix chainable 1,mult
di prefix prefix 2,mult
do prefix chainable 2,mult
bis prefix kis 2,mult
tri prefix chainable 3,mult
tris prefix kis 3,mult
tetr|tetra prefix chainable 4,mult
pent|penta prefix chainable 5,mult
hex|hexa prefix chainable 6,mult
hept|hepta prefix chainable 7,mult
oct|octa prefix chainable 8,mult
non|nona prefix chainable 9,mult
dec|deca prefix chainable 10,mult
undec|undeca prefix prefix 11,mult
eicos|eicosa|icos|icosa|ccs|cosa prefix chainable 20,mult
uneicos|uneicosa|unicos|uricosa prefix prefix 21,mult
triacont|triaconta|tricont|triconata prefix chainable 30,mult
tetracont|tetraconta prefix chainable 40,mult
pentacont|pentaconta prefix chainable 50,mult
hexacont|hexaconta prefix chainable 60,mult
heptacont|heptaconta prefix chainable 70,mult
octacont|octaconta prefix chainable 80,mult
nonacont|nonaconta prefix chainable 90,mult
hect|hecta prefix chainable 100,mult
dict|dicta prefix chainable 200,mult
trict|tricta prefix chainable 300,mult
tetract|tetract prefix chainable 400,mult
pentact|pentacta prefix chainable 500,mult
hexact|hexact prefix chainable 600,mult
heptact|heptacta prefix chainable 700,mult
octact|octacta prefix chainable 800,mult
nonact|nonacta prefix chainable 900,mult
kili|kilia prefix chainable 1000,mult
dili|dilia prefix chainable 2000,mult
trili|trilia prefix chainable 3000,mult
tetrali|tetralia prefix chainable 4000,mult
pentali|pentalia prefix chainable 5000,mult

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hexali|hexalia prefix chainable 6000,mult
 heptali|heptalia prefix chainable 7000,mult
 octali|octalia prefix chainable 8000,mult
 nonali|nonalia prefix chainable 9000,mult
 cyclo cyclo cyclo 1,cyclo
 spiro spiro unknown 1,spiro

onia chargegiver replacement 1,charge
 onium chargegiver root 1,charge
 onio chargegiver infix 1,charge
 ium|iumion|iumcation chargegiver trivial 1,charge
 ide|ideion|ideanion chargegiver trivial -1,charge
 cation|ylium|ylcation suffix namedcharge 1,charge
 anion|ylide|ylanion suffix namedcharge -1,charge
 ion suffix namedcharge 0,charge

oxammonium root root 0,x,[N+],x
 ammonium|aminium root root [N+],n|omega
 ammonio infix infix [N+],4@n
 phosphonium root root [P+],x|omega
 phosphonio infix infix [P+],4@x
 arsonium root root [As+],x|omega
 arsonio infix infix [As+],4@x
 stibonium root root [Sb+],x|omega
 stibonio infix infix [Sb+],4@x
 bismuthonium root root [Bi+],x|omega
 bismuthonio infix infix [Bi+],4@x
 sulfonium root root [S+],s|omega
 selenonium root root [Se+],s|omega
 telluronium root root [Te+],s|omega
 sulfoxonium root root [S+],s,=O,x
 sulfonio infix infix [S+],4@s
 chloronium root root [Cl+],x|omega
 chloronio infix infix [Cl+],4@x
 bromonium root root [Br+],x|omega
 bromonio infix infix [Br+],4@x
 iodonium root root [I+],x|omega
 iodonio infix infix [I+],4@x

actina replacement replacement [Ac],x
 alumina|alumin replacement replacement [Al],x
 argenta|argent replacement replacement [Ag],x
 arsa|ars|arsen replacement replacement [As],x
 arsora|arsor replacement replacement [AsH5],x
 astata|astat replacement replacement [At],x
 aura replacement replacement [Au],x
 aza|az replacement replacement N,n
 bara replacement replacement [Ba],x
 berkela|berkel replacement replacement [Bk],x
 berylla|beryll replacement replacement [Be],x
 bisma|bism replacement replacement [Bi],x
 bora|bor replacement replacement [B],x
 broma replacement replacement [Br],x
 cadma|cadm replacement replacement [Cd],x
 calca|calc replacement replacement [Ca],x
 californa|californ replacement replacement [Cf],x
 carba|carb replacement replacement [C],x

cera|cer replacement replacement [Ce],x
 chlora|replacement replacement [Cl],x
 chroma|chrom replacement replacement [Cr],x
 cobalta|replacement replacement [Co],x
 cupra|cupr replacement replacement [Cu],x
 cura|replacement replacement [Cm],x
 dysprosa|dyspros replacement replacement [Dy],x
 einsteina|einstein replacement replacement [Es],x
 europa|europ replacement replacement [Eu],x
 ferma|ferm replacement replacement [Fm],x
 ferra|ferr replacement replacement [Fe],x
 fluora|replacement replacement [F],x
 gadolina|gadol replacement replacement [Gd],x
 galla|replacement replacement [Ga],x
 germa|germ|german replacement replacement [Ge],x
 hafna|hafn replacement replacement [Hf],x
 holma|holm replacement replacement [Ho],x
 inda|replacement replacement [In],x
 ioda|replacement replacement [I],x
 irida|irid replacement replacement [Ir],x
 lanthana|lanthan replacement replacement [La],x
 lawrenca|lawrenc replacement replacement [Lr],x
 luteta|lutet replacement replacement [Lu],x
 magnesa|magnes replacement replacement [Mg],x
 mangana|mangan replacement replacement [Mn],x
 mendeleva|mendelev replacement replacement [Md],x
 mercura|mercur replacement replacement [Hg],x
 molybda|molybd replacement replacement [Mo],x
 neodyma|neodym replacement replacement [Nd],x
 neptuna|neptun replacement replacement [Np],x
 nickela|replacement replacement [Ni],x
 nioba|niob replacement replacement [Nb],x
 nobela|nobel replacement replacement [No],x
 osma|osm replacement replacement [Os],x
 oxa|ox replacement replacement O,x
 pallada|pallad replacement replacement [Pd],x
 phospho|phosph replacement replacement P,x
 phosphora|phosphor replacement phosphor [PH5],x
 platina|platin replacement replacement [Pt],x
 plumba|plumb replacement replacement [Pb],x
 plutona|pluton replacement replacement [Pu],x
 polona|polon replacement replacement [Po],x
 praseodyma|praseodym replacement replacement [Pr],x
 prometha|prometh replacement replacement [Pm],x
 protactina|protactin replacement replacement [Pa],x
 rada|replacement replacement [Ra],x
 rhena|rhen replacement replacement [Re],x
 rhoda|replacement replacement [Rh],x
 ruthena|ruthen replacement replacement [Ru],x
 samara|samar replacement replacement [Sm],x
 scanda|scand replacement replacement [Sc],x
 selena|selen replacement replacement [Se],x
 sila|sil|silic replacement replacement [Si],x
 stanna|stann replacement replacement [Sn],x
 stiba|stib|antimon replacement replacement [Sb],x
 stibora|stibor replacement replacement [SbH5],x
 stronta|stront replacement replacement [Sr],x

tantala|tantal replacement replacement [Ta],x
 techneta|technet replacement replacement [Tc],x
 tellura|tellur replacement replacement [Te],x
 terba|terb replacement replacement [Tb],x
 thalla|thall replacement replacement [Tl],x
 thia|thi replacement replacement S,x
 thora|thor replacement replacement [Th],x
 thula|thul replacement replacement [Th],x
 titana|titan replacement replacement [Ti],x
 tungsta|tungst|wolframa|wolfram replacement replacement [W],x
 urana|uran replacement replacement [U],x
 vanada|vanad replacement replacement [V],x
 ytterba|ytterb replacement replacement [Yb],x
 yttra|yttr replacement replacement [Y],x
 zinca|zinc replacement replacement [Zn],x
 zircona|zircon replacement replacement [Zr],x

 zirconyl|zirconyliv root setvalence [Zr++],x,(=O),x
 vanadyliv|vanadyl root setvalence [V++],x,(=O),x
 chromyl root setvalence [Cr++],x,(=O)(=O),x
 uranyl root setvalence [U++],x,(=O)(=O),x

 seleno|selen thio unknown [Se],x
 telluro|tellur thio unknown [Te],x
 thio|thi thio unknown S,x
 i|iso tert iso 3,tert
 sec tert sec 3,tert
 s tert sec 4,tert
 neo tert neo 4,tert
 t|tert|tertiary tert tert 4,tert
 imide|imid imide root N,n
 imido|imidyl imide root N,4@n
 chlorimide|chlorimid imide root NCl,x
 imide root oxime N,8@n
 chlorimide|chlorimid root oxime NCl,8@x
 hexafluorophosphoricacid root root [H+].[P-](F)(F)(F)(F)(F)F,x
 hexafluorosilicicacid root root [H+].[H+].[Si--](F)(F)(F)(F)(F)F,x
 tetrafluoroboricacid root root [H+].[B-](F)(F)(F)F,x
 hexafluorozirconicacid root root [H+].[H+].[Zr--](F)(F)(F)(F)(F)F,x
 nitramin cyanic cyanic N,1@x,[N+](=O)[O-],x
 isocyan cyanic cyanic N,1@x,=C=O,x
 isothiocyan cyanic cyanic N,1@x,=C=S,x
 isoselenocyan cyanic cyanic N,1@x,=C=[Se],x
 cyan cyanic cyanic O,1@x,C#N,x
 hydrocyan cyanic cyanic [H]C#N,x
 fulmin cyanic cyanic O,1@x,[N+]#[C-],x
 hydrofluor cyanic cyanic [H]F,x
 hydrochlor cyanic cyanic [H]Cl,x
 hydrobrom cyanic cyanic [H]Br,x
 hydroiod|hydriod cyanic cyanic [H]I,x
 tetron cyanic cyanic O,1, Ring, Ring1, C, 2, (=O), x, C, 3, C, 4, (=O), x, C, 5, Ring, Ring1
 osm cyanic cyanic [Os](=O)(=O)(=O)=O,x
 xanth|xanthogen cyanic cyanic O,x,C,x,(=,x,S,x,),x,S,s|w|omega
 rhodanin cyanic cyanic
 S,1, Ring, Ring1, C, 2, (=,x,S,x,),x,N,3,C,4,(=,x,O,x,),x,C,5, Ring, Ring1
 ellag cyanic cyanic O=C3Oc1c(O)c(O)cc4c1c2c(OC4=O)c(O)c(O)cc23,x

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ur cyanic cyanic
N,1, Ring, Ring1, C, 2, (=O), x, N, 3, C, 4, Ring, Ring2, N, 9, C, 8, (=O), x, N, 7, C, 5, =, x, Ring, Ring2, C, 6, (=O), x, Ring, Ring1
squar|quadrat cyanic cyanic
O,1@x,C,x, Ring, Ring1, =, x, C, x, (, x, O, 1@x, ), x, C, x, (=O), x, C, x, (=O), x, Ring, Ring1
crocon cyanic cyanic
O,1@x,C,x, Ring, Ring1, =, x, C, x, (, x, O, 1@x, ), x, C, x, (=O), x, C, x, (=O), x, C, x, (=O), x, Ring, Ring1
dehydroacet cyanic cyanic CC(C(C1=O)C(C=C(C)O1)=O)=O,x
ascorb|lascorb|ascorbyl|lascorbyl|isoascorb pseudosugar unknown x,x
ascorb|lascorb cyanic cyanic
O,x,C,3, Ring, Ring1, [C@@H], 4, (, x, [C@@H], 5, (, x, O, x, ), x, C, 6, O, x, ), x, O, x, C, 1, (=O), x, C, 2, (, x, O, x, ), x, =, x, Ring, Ring1
ascorbyl|lascorbyl root root
O,x,C,3, Ring, Ring1, [C@@H], 4, (, x, [C@@H], 5, (, x, O, x, ), x, C, 6, O, x, ), x, O, x, C, 1, (=O), x, C, 2, (, x, O, x, ), x, =, x, Ring, Ring1
isoascorb cyanic cyanic
O,x,C,3, Ring, Ring1, [C@@H], 4, (, x, [C@@H], 5, (, x, O, x, ), x, C, 6, O, x, ), x, O, x, C, 1, (=O), x, C, 2, (, x, O, x, ), x, =, x, Ring, Ring1
koj cyanic cyanic
o,1, Ring, Ring1, c, 2, c, 3, (O), x, c, 4, (=O), x, c, 5, c, 6, (CO), x, Ring, Ring1
picrolon cyanic cyanic O=C1N(C2=CC=C([N+])([O-])=O)C=C2)N=C(C)C1[N+])([O-])=O,x
barbitur cyanic cyanic
N,1@1, Ring, Ring1, C, 2, (=, x, O, x, ), x, N, 1@3, C, 4, (=, x, O, x, ), x, C, 5, C, 6, (=, x, O, x, ), x, Ring, Ring1
violur cyanic cyanic
N,1@1, Ring, Ring1, C, 2, (=, x, O, x, ), x, N, 1@3, C, 4, (=, x, O, x, ), x, C, 5, (=NO), x, C, 6, (=, x, O, x, ), x, Ring, Ring1
isobarbitur cyanic cyanic
n,1, Ring, Ring1, c, 2, (, x, O, 1@x, ), x, n, 3, c, 4, c, 5, (, x, O, 1@x, ), x, c, 6, (, x, O, 1@x, ), x, Ring, Ring1
cyanur cyanic cyanic
n,1, Ring, Ring1, c, 2, (, x, O, 1@x, ), x, n, 3, c, 4, (, x, O, 1@x, ), x, n, 5, c, 6, (, x, O, 1@x, ), x, Ring, Ring1
isocyanur cyanic cyanic
N,1@1, Ring, Ring1, C, 2, (=, x, O, x, ), x, N, 1@3, C, 4, (=, x, O, x, ), x, N, 1@5, C, 6, (=, x, O, x, ), x, Ring, Ring1
melanur cyanic cyanic
n,1, Ring, Ring1, c, 2, (, x, O, 1@x, ), x, n, 3, c, 4, (, x, O, 1@x, ), x, n, 5, c, 6, (, x, N, 1@x, ), x, Ring, Ring1
rhodizon cyanic cyanic
C,1, Ring, Ring1, (, x, O, 1@x, ), x, =, x, C, 2, (, x, O, 1@x, ), x, C, 3, (=O), x, C, 4, (=O), x, C, 5, (=O), x, C, 6, (=O), x, Ring, Ring1
chloranil cyanic cyanic
c,1, Ring, Ring1, (=O), x, c, 2, (Cl), x, c, 3, (, x, O, 1@x, ), x, c, 4, (=O), x, c, 5, (Cl), x, c, 6, (, x, O, 1@x, ), x, Ring, Ring1
bromanil cyanic cyanic
c,1, Ring, Ring1, (=O), x, c, 2, (Br), x, c, 3, (, x, O, 1@x, ), x, c, 4, (=O), x, c, 5, (Br), x, c, 6, (, x, O, 1@x, ), x, Ring, Ring1
bromanil root root
c,1, Ring, Ring1, (=O), x, c, 2, (Br), x, c, 3, (Br), x, c, 4, (=O), x, c, 5, (Br), x, c, 6, (Br), x, Ring, Ring1
nitranil cyanic cyanic c,1, Ring, Ring1, (=O), x, c, 2, ([N+])([O-])=O), x, c, 3, (, x, O, 1@x, ), x, c, 4, (=O), x, c, 5, ([N+])([O-])=O), x, c, 6, (, x, O, 1@x, ), x, Ring, Ring1
picr cyanic cyanic O,1@x,c,1, Ring, Ring1, c, 2, ([N+])([O-])=O), x, c, 3, c, 4, ([N+])([O-])=O), x, c, 5, c, 6, ([N+])([O-])=O), x, Ring, Ring1

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picryl root root c,4@1, Ring, Ring1, c, 2, ([N+]([O-])=O), x, c, 3, c, 4, ([N+]([O-])=O), x, c, 5, c, 6, ([N+]([O-])=O), x, Ring, Ring1
styphn cyanic cyanic O,1@x, c, 1, Ring, Ring1, c, 2, ([N+]([O-])=O), x, c, 3, (, x, O, 1@x, ), x, c, 4, ([N+]([O-])=O), x, c, 5, c, 6, ([N+]([O-])=O), x, Ring, Ring1
pyrophosphor cyanic cyanic
P, x, (=O), x, (, x, O, 1@x, ), x, (, x, O, 1@x, ), x, O, x, P, x, (=O), x, (, x, O, 1@x, ), x, O, 1@x
dithiopyrophosphor cyanic cyanic
P, x, (=S), x, (, x, O, 1@x, ), x, (, x, O, 1@x, ), x, O, x, P, x, (=S), x, (, x, O, 1@x, ), x, O, 1@x
peroxydisulf cyanic cyanic
S, x, (=O)(=O), x, (, x, O, 1@x, ), x, O, O, x, S, x, (=O)(=O), x, O, 1@x
pyrosulf cyanic cyanic S, x, (=O)(=O), x, (, x, O, 1@x, ), x, O, x, S, x, (=O)(=O), x, O, 1@x
isethion cyanic cyanic O,1@x, S, x, (=O)(=O), x, C, 1, C, 2, O, o
hydrosulfite|dithionite root root S, x, (=O), x, (, x, [O-], x, ), x, S, x, (=O), x, [O-], x
dithionate root root S, x, (=O)(=O), x, (, x, [O-], x, ), x, S, x, (=O)(=O), x, [O-], x
cacodyl cyanic cyanic [As](=O)(, x, O, 1@x, ) (C)C, x
chromotrop cyanic cyanic
c, 4, Ring, Ring1, c, 3, (S(=O)(=O), x, O, 1@x, ), x, c, 2, c, 1, (O), x, c, 8a, Ring, Ring2, c, 8, (O),
x, c, 7, c, 6, (S(=O)(=O), x, O, 1@x, ), x, c, 5, c, 4a, Ring, Ring1, Ring, Ring2
acid endercyanic unknown x, x
ochloranil root root
c, 1, Ring, Ring1, (=O), x, c, 2, (=O), x, c, 3, (Cl), x, c, 4, (Cl), x, c, 5, (Cl), x, c, 6, (Cl), x, Rin
g, Ring1
mchloranil root root
c, 1, Ring, Ring1, (=O), x, c, 2, (Cl), x, c, 3, (=O), x, c, 4, (Cl), x, c, 5, (Cl), x, c, 6, (Cl), x, Rin
g, Ring1
pchloranil|spergon root root
c, 1, Ring, Ring1, (=O), x, c, 2, (Cl), x, c, 3, (Cl), x, c, 4, (=O), x, c, 5, (Cl), x, c, 6, (Cl), x, Rin
g, Ring1
ate organometallicanion ate x, x
icacid|oicacid acid acid O,8@x, ., x, O, 5@x
ate|oate acid ate O,8@x, ., x, O, 5@x
ic|oic acid ic O,8@x, ., x, C, 5@x
ous acid ous O,5@x
ite acid ite O,5@x
amido acid infix O,8@x, ., x, N, 5@n
amido part2acid infix N,5@n
acid part2acid acid O,5@x
amide|amid part2acid amide N,6@n
amide|amid acid acid O,8@x, ., x, N, 6@n
chloramide|chloramid part2acid amide N,5@n, Cl, x
bromamide|bromamid part2acid amide N,5@n, Br, x
amidine|amidin|imidamide acid acid N,9@n' |n2, ., x, N, 6@n |n1
amidrazone|amidrazon acid acid N,9@n' , ., x, N, 5@n |n1, N, 2@n' |n2
hydrazide|hydrazid|ohydrazide|ohydrazid acid acid
O,8@x, ., x, N, 5@n |1 |n1, N, 2@n' |2 |n2
hydrazide|hydrazid part2acid amide N,5@n |1 |n1, N, 2@n' |2 |n2
onitrile|nitrile acid nitrile N,12@x
nitrile|anammonide part2acid nitrile N,12@x
ether part2acid acid O,4@x, C, x, C, x
oyl acid makefree O,8@x
basic basic unknown [H],4@x
aldehyde|aldehyd part2acid acid H,4@x
aldehyde|aldehyd|al acid acid O,8@x, ., x, H, 4@x
aldoxime|aldoxim acid acid H,4@x, ., x, N, 8@x, O, o
aldimine|aldimin acid acid H,4@x, ., x, N, 8@n
lacton|lactone part2acid lactone O,5@x

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thiolacton|thiolactone part2acid lactone S,5@x
selenolacton|selenolactone part2acid lactone [Se],5@x
tellurolacton|tellurolactone part2acid lactone [Te],5@x
lacton|lactone|olacton|olactone|iclacton|iclactone|olide|olid acid lactone
O,8@x,.,x,O,5@x
lactam part2acid lactone N,5@x
lactam|olactam|iclactam acid lactone O,8@x,.,x,N,5@x
lactim part2acid lactone N,9@x
lactim|olactim|iclactim acid lactone O,4@x,.,x,N,9@x
sulfimide part2acid lactone N,4@x,S,1@x,(=O)(=O),x
anilide|analide acid acid
O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),
x
anilide|analide part2acid amide
N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),x
anilido|analido acid infix
O,8@x,.,x,N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),
x
anilido|analido part2acid infix
N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),x
4nitroanilide|pnitroanilide acid acid
O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1),x
4nitroanilide|pnitroanilide part2acid acid
N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1),x
morpholide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
morpholide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
ophenone acid acid
O,8@x,.,x,c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
ophenone part2acid acid
c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
onaphthone acid acid
O,8@x,.,x,c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',
c,8a',Ring,Ring1,Ring,Ring2
onaphthone part2acid acid
c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',c,8a',Ring
,Ring1,Ring,Ring2
ureide acid acid O,8@x,.,x,N,4@n,C(=O),x,N,n'
ureide part2acid amide N,4@n,C(=O),x,N,n'
piperazide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperazide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperidide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
piperidide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
anhydride|cyclicanhydride part2acid anhydride O,5@x
thioanhydride part2acid anhydride S,5@x
selenoanhydride part2acid anhydride [Se],5@x
telluroanhydride part2acid anhydride [Te],5@x
imid|imide part2acid anhydride N,5@x
cyclam root root S,x,(=O)(=O),x,(NC1CCCC1),x,O,1@x
atrop loveracid root
C,x,C,x,(,x,=,x,C,x),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
pinon loveracid root CCC1CC(C(C)(C)1)C(=O)C,x
benzil loveracid root
C,x,C,a|alpha,(,x,O,x),x,(,x,c,1,Ring,Ring1,=,x,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,
),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2

glycoll|glycol leveracid alkane C,x,C,2|w|omega,O,x
thioglycoll|thioglycol leveracid root C,x,C,2,S,w|omega
selenoglycoll|selenoglycol leveracid root C,x,C,2,[Se],w|omega
telluroglycoll|telluroglycol leveracid root C,x,C,2,[Te],w|omega
boro|bor|orthobor leveracid root [B],x,(,x,O,1@o''),x,(,x,O,1@o'),x,O,1@o
metabor leveracid root [B],x,(,x,=,x,O,o'),x,O,1@o
perbor leveracid root [B],x,(,x,=,x,O,x),(,x,=,x,O,x),x,O,1@o
borin leveracid root [B],x,O,1@o
borono|boron leveracid counterion [B],4@x,(,x,O,1@o'),x,O,1@o
diphosphor|pyrophosphor|pyrophosph leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''|p2),x,O,1@o''''
dithiodiphosphor|dithiopyrophosphor|dithiopyrophosph leveracid root
P,a|alpha,(=,x,S,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,S,x),(,x,O,1@o''|p2),x,O,1@o''''
phosphosulf leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,O,x,S,b|beta,(=,x,O,x),(=,x,O,x),x,O,1@o''''
glycerophosph|alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalpha
glycerophosph leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,OCC(O)CO,x
glycerophospho|alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dla
lphaglycerophospho leveracid root
P,4@a|alpha,(=,x,O,x),(,x,O,1@o'),x,OCC(O)CO,x
triphosphor leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''|p2),x,O,x,P,g|gamma,(=,x,O,x),(,x,O,1@o''''|p3),x,O,1@o''''''|p3
2thiodiphosphor leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,S,x),(,x,O,1@o''|p2),x,O,1@o''''
3thiotriphosphor leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''|p2),x,O,x,P,g|gamma,(=,x,S,x),(,x,O,1@o''''|p3),x,O,1@o''''''|p3
tetraphosphor leveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'|p1),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''|p2),x,O,x,P,g|gamma,(=,x,O,x),(,x,O,1@o''''|p3),x,O,o''''''|p3,P,d|delta,(=,x,O,x),(,x,O,1@o''''''|p4),x,O,1@o''''''''|p4
phosphoro|phosphor|phosph|orthophosph|orthophosphor leveracid root
P,x,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,O,1@o
phosphono|phosphon leveracid counterion P,4@x,(=,x,O,x),(,x,O,1@o'),x,O,1@o
phospheno|phosphen leveracid root P,x,(=,x,O,x),(=,x,O,x),x,O,1@o
hypophosph leveracid root [PH0],x,(=,x,O,x),(=,x,O,x),x,O,1@o
phosphino|phosphin leveracid root [PH2],x,(=,x,O,x),x,O,1@o
phosphoenolpyruv leveracid root
P,x,(=,x,O,x),(,x,O,1@o'),(,x,O,1@o),x,O,x,C,x,(=C),x,C,x,(=O),x,O,1@x
phyt leveracid root
O=P(,x,O,1@x),(,x,O,1@x),O[C@H]1[C@@H](OP(,x,O,1@x),(,x,O,1@x)=O)[C@@H](OP(,x,O,1@x),(,x,O,1@x)=O)[C@H](OP(,x,O,1@x),(,x,O,1@x)=O)[C@@H](OP(,x,O,1@x),(,x,O,1@x)=O)[C@@H]1OP(,x,O,1@x),(,x,O,1@x)=O,x
orthoarsen|arseno|arsen leveracid root
[As],x,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,O,1@o
arsenicacid root root [As],x,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,O,1@o
arsono|arson leveracid counterion [As],4@x,(=,x,O,x),(,x,O,1@o'),x,O,1@o
arsino|arsin leveracid root [AsH2],x,(=,x,O,x),x,O,1@o
stibeno|stiben|antimon leveracid root
[Sb],x,(=,x,O,x),(,x,O,1@o''),(,x,O,1@o'),x,O,1@o
stibono|stibon leveracid counterion [Sb],4@x,(=,x,O,x),(,x,O,1@o'),x,O,1@o


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metanil loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,c,1, Ring, Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,
5,c,6, Ring, Ring1
metanilyl root root
S,4@x,(=,x,O,x,)(,x,=O,x,),x,c,1, Ring, Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,5,c,6, Ring
, Ring1
vanad|metavanad loveracid root [V],x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
orthovanad loveracid root [V],x,(=,x,O,x,)(,x,O,o'',)(,x,O,o'',),x,O,1@o
fluor loveracid root F,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
chlor loveracid root Cl,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
brom loveracid root Br,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
iod loveracid root I,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
metaperiod loveracid root I,x,(=,x,O,x,)(=,x,O,x,)(,x,=O,x,),x,O,1@o
paraperiod loveracid root
I,x,(=,x,O,x,)(,x,O,1@o'''''),(,x,O,1@o'''''),(,x,O,1@o'''),(,x,O,1@o'),x,O,1@o
semialdehyde tailderiverdiacid acid H,4@x
aldehyd deriverdiacid acid O,8@x,,x,H,4@x
am deriverdiacid acid O,8@x,,x,N,6@n
anil deriverdiacid acid
O,8@x,,x,N,4@n,c,x, Ring, Ring1,c,2',c,3',c,4',c,5',c,6', Ring, Ring1
bromo|brom deriveracid loveracidderiver Br,4@x
chloro|chlor deriveracid loveracidderiver Cl,4@x
fluoro|fluor deriveracid loveracidderiver F,4@x
cyano deriveracid loveracidderiver C,4@x,#N,x
iodo|iod deriveracid loveracidderiver I,4@x
amido|amid deriveracid loveracidderiver N,6@n
anilido deriveracid loveracidderiver
N,4@n,c,x, Ring, Ring1,c,2,c,3,c,4,c,5,c,6, Ring, Ring1
morpholino deriveracid loveracidderiver
N,4@x, Ring, Ring1,C,x,C,x,O,x,C,x,C,x, Ring, Ring1
azido|azid deriveracid loveracidderiver N,4@x,=[N+]=[N-],x
bromido|bromid deriveracid acid Br,4@x
bromo|brom deriveracid loveracidderiver Br,4@x
chlorido|chlorid deriveracid acid Cl,4@x
choro|chlor deriveracid loveracidderiver Cl,4@x
cyanatido|cyanatid deriveracid acid O,4@x,C#N,x
cyanido|cyanid deriveracid acid C,4@x,#N,x
cyano deriveracid loveracidderiver C,4@x,#N,x
fluorido|fluorid deriveracid acid F,4@x
fluoro|fluor deriveracid loveracidderiver F,4@x
hydroxam|ohydroxam deriveracid acid N,5@n,O,x
hydroxim|ohydroxim deriveracid acid N,8@n,O,x
hydrazon|ohydrazon deriveracid acid N,8@x,N,n
iodido|iodid deriveracid acid I,4@x
iodo|iod deriveracid loveracidderiver I,4@x
isocyanatido|isocyanatid deriveracid acid N,4@x,=C=O,x
isocyanido|isocyanid deriveracid acid [N+],4@x,#[C-],x
thiocyanatido|thiocyanatid deriveracid acid S,4@x,C#N,x
isothiocyanatido|isothiocyanatid deriveracid acid N,4@x,=C=S,x
imido|imid deriveracid acid N,8@n
hydrazido|hydrazid deriveracid acid N,5@n|1',N,2@n'|2'
peroxo|perox|peroxy deriveracid acid O,4@x,O,1@oo
dithioperoxy deriveracid acid S,4@x,S,1@ss
seleno|selen deriveracid acid [Se],8@se
telluro|tellur deriveracid acid [Te],8@te
thio|thi|thion|thiono deriveracid acid S,8@S
thiolo|thiol deriveracid acid S,5@s

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per peracid peracid x,x
hypo peracid hypoacid x,x
etine|etin|etene|eten heterocyc oline C,1, Ring, Ring1, C,2, C,3, C,4, Ring, Ring1
oline|olin|olene|olen heterocyc oline C,1, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
isoxazoline|isoxazolin|isoazoline|isoazolin root oline
O,1, Ring, Ring1, N,2, C,3, C,4, C,5, Ring, Ring1
isothiazoline|isothiazolin root oline S,1, Ring, Ring1, N,2, C,3, C,4, C,5, Ring, Ring1
isoselenazoline|isoselenazolin root oline
[se],1, Ring, Ring1, N,2, C,3, C,4, C,5, Ring, Ring1
pyrroline|pyrrolin root oline N,1, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
pyrazoline|pyrazolin root oline N,1, Ring, Ring1, N,2, C,3, C,4, C,5, Ring, Ring1
pyrazolino root oline N,4@1, Ring, Ring1, N,2, C,3, C,4, C,5, Ring, Ring1
imidazoline|imidazolin root oline C,2, Ring, Ring1, N,3, C,4, C,5, N,1, Ring, Ring1
sulfolene|sulfolen root oline
S,1, (=,x,O,x,) (=,x,O,x,) x, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
sulfol root root
S,1, (=,x,O,x,) (=,x,O,x,) x, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
iridine|iridin heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, Ring, Ring1
etidine|etidine heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, C,4, Ring, Ring1
olidine|olidin|olid heterocyc heterocyc
C,1, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
irene|irine|irin|iren heterocyc heterocyc c,1, Ring, Ring1, c,2, c,3, Ring, Ring1
ireno|irino|irin|iren opfuser heterocyc c,1, Ring, Ring1, c,2, c,3, Ring, Ring1
irane|iran heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, Ring, Ring1
ete|et heterocyc heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, Ring, Ring1
eto opfuser heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, Ring, Ring1
etane|etan heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, C,4, Ring, Ring1
ole|ol heterocyc heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, c,5, Ring, Ring1
olo opfuser heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, c,5, Ring, Ring1
olane|olan heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, C,4, C,5, Ring, Ring1
ine|in heterocyc ine
c,1, Ring, Ring1, c,2|o|ortho, c,3|m|meta, c,4|p|para, c,5, c,6, Ring, Ring1
ino opfuser ine c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, Ring, Ring1
inine|inin heterocyc inine
c,1, Ring, Ring1, c,2|o|ortho, c,3|m|meta, c,4|p|para, c,5, c,6, Ring, Ring1
ane|an heterocyc ane
C,1, Ring, Ring1, C,2|o|ortho, C,3|m|meta, C,4|p|para, C,5, C,6, Ring, Ring1
inane|inan heterocyc inan
C,1, Ring, Ring1, C,2|o|ortho, C,3|m|meta, C,4|p|para, C,5, C,6, Ring, Ring1
epane|epan heterocyc heterocyc C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, C,7, Ring, Ring1
epine|epin heterocyc heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, Ring, Ring1
epino opfuser heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, Ring, Ring1
ocane|ocan heterocyc heterocyc
C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, C,7, C,8, Ring, Ring1
ocine|ocin heterocyc heterocyc
c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, c,8, Ring, Ring1
ocino opfuser heterocyc c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, c,8, Ring, Ring1
onane|onan heterocyc heterocyc
C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, Ring, Ring1
online|onin heterocyc heterocyc
c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, c,8, c,9, Ring, Ring1
onino opfuser heterocyc
c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, c,8, c,9, Ring, Ring1
ecane|ecan heterocyc heterocyc
C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, C,10, Ring, Ring1
ecine|ecin heterocyc heterocyc
c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,7, c,8, c,9, c,10, Ring, Ring1

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ecino|ecin opfuser heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, Ring, Ring1
cyclodecine|cycloundecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, Ring, Ring1
cycloundecine|cycloundecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, Ring, Ring1
cyclododecine|cyclododecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, Ring, Ring1
cyclotridecine|cyclotridecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, Ring, Ring1
cyclotetradecine|cyclotetradecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, Ring, Ring1
cyclopentadecine|cyclopentadecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, c, 15, Ring, Ring1
cyclohexadecine|cyclohexadecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, c, 15, c, 16, Ring, Ring1
cycloheptadecine|cycloheptadecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, c, 15, c, 16, c, 17, Ring, Ring1
cyclooctadecine|cyclooctadecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, c, 15, c, 16, c, 17, c, 18, Ring, Ring1
cyclononadecine|cyclononadecin heterocyc heterocyc
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, c, 7, c, 8, c, 9, c, 10, c, 11, c, 12, c, 13, c, 14, c, 15, c, 16, c, 17, c, 18, c, 19, Ring, Ring1
salt|salts|deriv|derivative salt unknown x,x
saltof salt saltof x,x
ester|esters ester unknown x,x
esterswith|estersof|esterwith|esterof ester esterwith x,x
ylene|ylen|ylenediyl ylene ylene x,x
0 roman unknown 0,x
i|1+|+1 roman unknown 1,x
ii|2+|+2 roman unknown 2,x
iii|3+|+3 roman unknown 3,x
iv|4+|+4 roman unknown 4,x
v|5+|+5 roman unknown 5,x
vi|6+|+6 roman unknown 6,x
vii|7+|+7 roman unknown 7,x
viii|8+|+8 roman unknown 8,x
ix|9+|+9 roman unknown 9,x
h hydroh unknown [H],4@x
hydro root hydroroot [H],4@x
annulene annulene unknown x,x
crown crown unknown x,x
cis+trans unknown unknown x,x
vitamin unknown unknown x,x
support unknown unknown x,x
deposition unknown unknown x,x
tion|ition unknown unknown x,x
electron unknown unknown x,x
pesticide unknown unknown x,x
16n|15n|14n nothandled nothandled x,x
99m nothandled nothandled x,x
nonoxynol nothandled nothandled x,x

kition nothandled nothandled x,x
 resinol nothandled nothandled x,x
 mersol nothandled nothandled x,x
 american nothandled nothandled x,x
 turmeric nothandled nothandled x,x
 phenacid|phenacide nothandled nothandled x,x
 sulfurized nothandled nothandled x,x
 branched nothandled nothandled x,x
 carbor nothandled nothandled x,x
 cuproxoline nothandled nothandled x,x
 dioxygenyl nothandled nothandled x,x
 cyclodextrin nothandled nothandled x,x
 octapren|hexapren|undecapren nothandled nothandled x,x
 oato|ato nothandled nothandled x,x
 camphorato|camphorate nothandled nothandled x,x
 acetanide nothandled nothandled x,x
 alcoholate nothandled nothandled x,x
 cyclobutoic nothandled nothandled x,x
 fucoidan nothandled nothandled x,x
 margarite nothandled nothandled x,x
 pyrite nothandled nothandled x,x
 glycerite nothandled nothandled x,x
 pyroxylin nothandled nothandled x,x
 cosmoline|cosmetol nothandled nothandled x,x
 cupricol|cuproxol nothandled nothandled x,x
 alol nothandled nothandled x,x
 prenolone nothandled nothandled x,x
 cergona nothandled nothandled x,x
 platinol nothandled nothandled x,x
 antin nothandled nothandled x,x
 germanin nothandled nothandled x,x
 phosphomolyb nothandled nothandled x,x
 anhydro nothandled nothandled x,x
 base nothandled nothandled x,x
 thioflavin|thioflavine nothandled nothandled x,x
 dionate|dionato nothandled nothandled x,x
 doxyl nothandled nothandled x,x
 acetylacetanato nothandled nothandled x,x
 naphtholas nothandled nothandled x,x
 compounded nothandled nothandled x,x
 ketopinic nothandled nothandled x,x
 indoxyl nothandled nothandled x,x
 indo nothandled nothandled x,x
 sulfobetaine nothandled nothandled x,x
 coenzyme nothandled nothandled x,x
 chlorin nothandled nothandled x,x
 dehydro nothandled nothandled x,x
 benzothiolate nothandled nothandled x,x
 benzanthren nothandled nothandled x,x
 mg nothandled nothandled x,x
 vinglycin nothandled nothandled x,x
 calanolide nothandled nothandled x,x
 perbor nothandled nothandled x,x
 dionato|dionate|acetanate nothandled nothandled x,x
 tetraborate nothandled nothandled x,x
 mefluide nothandled nothandled x,x
 decavanadate nothandled nothandled x,x

benzin nothandled nothandled x,x
dodecin nothandled nothandled x,x
methin nothandled nothandled x,x
- nothandled nothandled x,x
tolane nothandled nothandled x,x
monocrotaline nothandled nothandled x,x
adiphenine nothandled nothandled x,x
anhydridewith nothandled nothandled x,x
terpin nothandled nothandled x,x
thiuram nothandled nothandled x,x
acaprazine nothandled unknown x,x
acaralate nothandled unknown x,x
acetazide nothandled unknown x,x
acetazolamide root root CC(NC1=NN=C(S(N)(=O)=O)S1)=O,x
acetene nothandled unknown x,x
acetohexamide nothandled unknown x,x
acetonyl nothandled unknown x,x
aconitine nothandled unknown x,x
alipamide nothandled unknown x,x
ambrosin nothandled unknown x,x
amygdalin nothandled unknown x,x
anisene nothandled unknown x,x
anisindione nothandled unknown x,x
antichlor nothandled unknown x,x
antiethanol nothandled unknown x,x
antiformin nothandled unknown x,x
antiphen nothandled unknown x,x
arsamin nothandled unknown x,x
arsenal nothandled unknown x,x
arsenolite nothandled unknown x,x
atolide nothandled unknown x,x
azamethone nothandled unknown x,x
azinthiamide nothandled unknown x,x
azobutyl nothandled unknown x,x
azolimine nothandled unknown x,x
azopyrin nothandled unknown x,x
benzilan nothandled unknown x,x
benzilen nothandled unknown x,x
benzole nothandled unknown x,x
benzolin nothandled unknown x,x
benzone nothandled unknown x,x
benzoxonium nothandled unknown x,x
benztropine|benzotropine root root CN3C4CC(CC3CC4)OC(C2=CC=CC=C2)C1=CC=CC=C1,x
biamine nothandled unknown x,x
bichlorendo nothandled unknown x,x
biclofibrate nothandled unknown x,x
biformylchlorazin nothandled unknown x,x
biphenate nothandled unknown x,x
bisoxypfen nothandled unknown x,x
blauramine nothandled unknown x,x
borolin nothandled unknown x,x
boroxine nothandled unknown x,x
bromacrylide nothandled unknown x,x
bromamide nothandled unknown x,x
bromethalin nothandled unknown x,x
bromhexine root root CN(C2CCCCC2)CC1=C(N)C(Br)=CC(Br)=C1,x
brominal nothandled unknown x,x

bromobutide nothandled unknown x,x
bromol nothandled unknown x,x
bromopropylate nothandled unknown x,x
bromoxanide nothandled unknown x,x
brompyrazon nothandled unknown x,x
butalamine nothandled unknown x,x
butamid nothandled unknown x,x
butethamine nothandled unknown x,x
butethanol nothandled unknown x,x
butoctamide nothandled unknown x,x
butonate nothandled unknown x,x
butone nothandled unknown x,x
butoxylate nothandled unknown x,x
butylenin nothandled unknown x,x
butylpyrin nothandled unknown x,x
calcion root root [O-]S(=O)(C1=CC(C=C(S([O-]))(=O)=O)C(N=NC4=CC(S([O-]))(=O)=O)=CC5=C4C=C(O)C=C5S([O-])(=O)=O)=C3O)=C3C(N=NC2=C(S([O-]))(=O)=O)C=C6C(C(O)=CC(S([O-]))(=O)=O)=C6)=C2O)=C1)O.[Na+].[Na+].[Na+].[Na+].[Na+].[Na+],x
camphorene nothandled unknown x,x
carbamine nothandled unknown x,x
carbamate nothandled unknown x,x
carbromal nothandled unknown x,x
carbutamide nothandled unknown x,x
carbylamine nothandled unknown x,x
cardiamid nothandled unknown x,x
cardiamine nothandled unknown x,x
cardiol nothandled unknown x,x
caryne nothandled unknown x,x
cetamid nothandled unknown x,x
chelidonine root root CN5CC1=C(C6C(CC4=CC3=C(C=C4C56)OC3)O)C=CC2=C1OC2O,x
chinacrin|chinacrine nothandled unknown x,x
chinoxform nothandled unknown x,x
chinoleine nothandled unknown x,x
chloralose nothandled unknown x,x
chlorazine nothandled unknown x,x
chlorbicyclen nothandled unknown x,x
chlorbisan nothandled unknown x,x
chlorbutol nothandled unknown x,x
chlorethate nothandled unknown x,x
chlorindan nothandled unknown x,x
chlorisopropamide nothandled unknown x,x
chlormethine nothandled unknown x,x
chloroazodian nothandled unknown x,x
chlorobutin nothandled unknown x,x
chloroepoxide nothandled unknown x,x
chloronaphthine nothandled unknown x,x
chloropropamide nothandled unknown x,x
chloropropylate nothandled unknown x,x
chloropyramine root root C1C1=CC=C(C=C1)CN(C2=CC=CC=N2)CCN(C)C,x
chlorothen nothandled unknown x,x
chlorothenylpyramine nothandled unknown x,x
chlorotrisin nothandled unknown x,x
chloroxylenol nothandled unknown x,x
chlorphenamine nothandled unknown x,x
chlortalidone nothandled unknown x,x
chlorthiamid nothandled unknown x,x

chlorthioamide nothandled unknown x,x
 cinchonamine nothandled unknown x,x
 cineol|cineole nothandled unknown x,x
 citralite nothandled unknown x,x
 citrene nothandled unknown x,x
 citronyl nothandled unknown x,x
 citrylone nothandled unknown x,x
 coniferin nothandled unknown x,x
 cresotine nothandled unknown x,x
 crotepoide nothandled unknown x,x
 crotonylene nothandled unknown x,x
 cupricin nothandled unknown x,x
 cyanogenamide nothandled unknown x,x
 cyclamen nothandled unknown x,x
 cyclobutyrol nothandled unknown x,x
 cyclopentamine nothandled unknown x,x
 cyclopentolate root root CN(CCOC(C(C2(CCCC2)O)C1=CC=CC=C1)=O)C,x
 daconit nothandled unknown x,x
 dazidamine nothandled unknown x,x
 decitropine nothandled unknown x,x
 delphinine nothandled unknown x,x
 diazan nothandled unknown x,x
 diazepam nothandled unknown x,x
 dibrompropamidine nothandled unknown x,x
 dibutin nothandled unknown x,x
 dichlordiphenprop nothandled unknown x,x
 dimethacrin nothandled unknown x,x
 dimethoxanate nothandled unknown x,x
 dimidazon nothandled unknown x,x
 diodoxylin nothandled unknown x,x
 dioxybenzone root root O=C(C2=CC=C(OC)C=C2O)C1=C(O)C=CC=C1,x
 diphenoxylate root root
 CCOC(C1(C4=CC=CC=C4)CCN(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C#N)CC1)=O,x
 diphenylpyraline root root CN1CCC(OC(C3=CC=CC=C3)C2=CC=CC=C2)CC1,x
 disilyln nothandled unknown x,x
 disobutamide nothandled unknown x,x
 dithiazanine nothandled unknown x,x
 dothiepin nothandled unknown x,x
 doxaminol nothandled unknown x,x
 doxaprost nothandled unknown x,x
 doxepin root root CN(C)CCC=C1C3=C(C=CC=C3)OCC2=C1C=CC=C2,x
 doxopin nothandled unknown x,x
 efuranol nothandled unknown x,x
 endocet nothandled unknown x,x
 endoiodin nothandled unknown x,x
 esorb nothandled unknown x,x
 estilben nothandled unknown x,x
 ethamide nothandled unknown x,x
 ethide nothandled unknown x,x
 ethinamide nothandled unknown x,x
 ethine nothandled unknown x,x
 ethionamide root root NC(C1=CC(CC)=NC=C1)=S,x
 ethoxazene nothandled unknown x,x
 ethylan nothandled unknown x,x
 ethylhexaldehyde nothandled unknown x,x
 etryptamine nothandled unknown x,x
 flavamine nothandled unknown x,x

fluoroformylone nothandled unknown x,x
fluoromethalone nothandled unknown x,x
fluorometholone nothandled unknown x,x
fluroxypyr nothandled unknown x,x
formamidoepoxide nothandled unknown x,x
formyldienolone nothandled unknown x,x
formylmethanofuran nothandled unknown x,x
fumarin nothandled unknown x,x
furalazine nothandled unknown x,x
furatoxin nothandled unknown x,x
furfurin nothandled unknown x,x
gallamine nothandled unknown x,x
glucid nothandled unknown x,x
glyoxyldiureide nothandled unknown x,x
gonacrine nothandled unknown x,x
hexamethylenetetraamine nothandled unknown x,x
hexylthiocarbam nothandled unknown x,x
hydantal nothandled unknown x,x
hydantin nothandled unknown x,x
hydantoinal nothandled unknown x,x
hydantol nothandled unknown x,x
iodamide nothandled unknown x,x
iodixanol nothandled unknown x,x
iodoxamic nothandled unknown x,x
isopropalin nothandled unknown x,x
isopropamide root root CC([N+](CCC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=O)(C(C)C)C)C,x
lactal nothandled unknown x,x
lactin nothandled unknown x,x
largon nothandled unknown x,x
laurenyne nothandled unknown x,x
laurine nothandled unknown x,x
lazo nothandled unknown x,x
lethane nothandled unknown x,x
leucol nothandled unknown x,x
lindane nothandled unknown x,x
lindol nothandled unknown x,x
lutidon nothandled unknown x,x
malonal nothandled unknown x,x
mesofolin nothandled unknown x,x
metachlorphenprop nothandled unknown x,x
methanopterine nothandled unknown x,x
methacetin nothandled unknown x,x
methacetone nothandled unknown x,x
methanofuran nothandled unknown x,x
metharsan nothandled unknown x,x
methazid nothandled unknown x,x
methazolamide root root CC(N=C1SC(S(N)(=O)=O)=NN1C)=O,x
methiodal nothandled unknown x,x
methionine nothandled unknown x,x
methoxychlor root root ClC(C1)(C1)C(C2=CC=C(OC)C=C2)C1=CC=C(OC)C=C1,x
methylaminopterine nothandled unknown x,x
methylenyl nothandled unknown x,x
methylone nothandled unknown x,x
monazan nothandled unknown x,x
monazol nothandled unknown x,x
monobenzene nothandled unknown x,x
montanine nothandled unknown x,x

morinamide nothandled unknown x,x
 naphthonone nothandled unknown x,x
 neonal nothandled unknown x,x
 neophan nothandled unknown x,x
 neraminol nothandled unknown x,x
 nicetal nothandled unknown x,x
 nicetamide nothandled unknown x,x
 nitralin nothandled unknown x,x
 nitrochlor nothandled unknown x,x
 nitroglycerin nothandled unknown x,x
 nitroglycerol nothandled unknown x,x
 octatropine nothandled unknown x,x
 ophthalmamin nothandled unknown x,x
 oxaine nothandled unknown x,x
 oxamyl nothandled unknown x,x
 oxanamide nothandled unknown x,x
 oxanilide nothandled unknown x,x
 oxanthrene nothandled unknown x,x
 oxolamine root root CCN(CCC1=NC(C2=CC=CC=C2)=NO1)CC,x
 oxophenarsine nothandled unknown x,x
 oxoprostol nothandled unknown x,x
 oxybutynin root root CCN(CC#CCOC(C(C1CCCCC1)(C2CCCCC2)O)=O)CC,x
 oxydiazol nothandled unknown x,x
 oxyfume nothandled unknown x,x
 oxylan nothandled unknown x,x
 oxylite nothandled unknown x,x
 pentalenene nothandled unknown x,x
 pentalenolactone nothandled unknown x,x
 pentanochlor nothandled unknown x,x
 pernittr nothandled unknown x,x
 persilic nothandled unknown x,x
 phenactropinium nothandled unknown x,x
 phenatine nothandled unknown x,x
 phenatoine nothandled unknown x,x
 phenazon nothandled unknown x,x
 phenformin root root N=C(NC(N)=N)NCCC1=CC=CC=C1,x
 phenonyl nothandled unknown x,x
 phenoxethol nothandled unknown x,x
 phenoxybenzamine nothandled unknown x,x
 phenoxytol nothandled unknown x,x
 phenvalerate nothandled unknown x,x
 phloretin root root O=C(CCC2=CC=C(O)C=C2)C1=C(O)C=C(O)C=C1O,x
 phosphaniline nothandled unknown x,x
 phosphetrol nothandled unknown x,x
 phosphotrienin nothandled unknown x,x
 phthalazolinol nothandled unknown x,x
 phytin nothandled unknown x,x
 pinacolin nothandled unknown x,x
 piperazate nothandled unknown x,x
 piperidolate root root O=C(OC2CN(CC)CCC2)C(C3=CC=CC=C3)C1=CC=CC=C1,x
 pivalone nothandled unknown x,x
 pivalyn nothandled unknown x,x
 propal nothandled unknown x,x
 propamidine nothandled unknown x,x
 propargite nothandled unknown x,x
 propazolamide nothandled unknown x,x
 propiodal nothandled unknown x,x

propon nothandled unknown x,x
proponal nothandled unknown x,x
pyramin nothandled unknown x,x
pyrazofurin nothandled unknown x,x
pyrazolynate nothandled unknown x,x
pyrazon nothandled unknown x,x
pyridate nothandled unknown x,x
pyridazol nothandled unknown x,x
pyridenal nothandled unknown x,x
pyridene nothandled unknown x,x
pyrinamine nothandled unknown x,x
pyroxychlor nothandled unknown x,x
pyroxyfur nothandled unknown x,x
razide nothandled unknown x,x
razoxane nothandled unknown x,x
razoxane nothandled unknown x,x
razoxin nothandled unknown x,x
restran nothandled unknown x,x
restryl nothandled unknown x,x
roxindole nothandled unknown x,x
roxion nothandled unknown x,x
saccharimide nothandled unknown x,x
serinal nothandled unknown x,x
shoxin nothandled unknown x,x
silantin nothandled unknown x,x
soxinol nothandled unknown x,x
stoxil nothandled unknown x,x
styron nothandled unknown x,x
sulfacid nothandled unknown x,x
sulfalene nothandled unknown x,x
sulfamethazine|sulfamethazin nothandled unknown x,x
sulfamethin nothandled unknown x,x
sulfodiazol nothandled unknown x,x
sulfurine nothandled unknown x,x
sulfurol nothandled unknown x,x
syncurine nothandled unknown x,x
synhexyl nothandled unknown x,x
synoestron nothandled unknown x,x
synpren nothandled unknown x,x
syringin nothandled unknown x,x
talon nothandled unknown x,x
tartran nothandled unknown x,x
terbolan nothandled unknown x,x
terbut nothandled unknown x,x
terbutaline nothandled unknown x,x
terbutol nothandled unknown x,x
teroxalene nothandled unknown x,x
tetralide nothandled unknown x,x
tetralite nothandled unknown x,x
tetrathiin nothandled unknown x,x
thenylchlor nothandled unknown x,x
thenylene nothandled unknown x,x
thenylpyramine nothandled unknown x,x
thiabenzazole nothandled unknown x,x
thiadenazonium nothandled unknown x,x
thiadiazinol nothandled unknown x,x
thiamylal root root S=C(N1)NC(C(C(C)CCC)(CC=C)C1=O)=O,x

thiazopyr nothandled unknown x,x
thioallate nothandled unknown x,x
thiocuran nothandled unknown x,x
thionylan nothandled unknown x,x
thioxamyl nothandled unknown x,x
thorazine nothandled unknown x,x
tolamide nothandled unknown x,x
tolamine nothandled unknown x,x
tolbutamide root root O=C(NS(C1=CC=C(C)C=C1)(=O)=O)NCCCC,x
tolcyclamide nothandled unknown x,x
tolite nothandled unknown x,x
tolnaphthate nothandled unknown x,x
tolpentamide nothandled unknown x,x
tolpropamine nothandled unknown x,x
transamine nothandled unknown x,x
triazbutyl nothandled unknown x,x
triazinate nothandled unknown x,x
tricinolon nothandled unknown x,x
tricurran nothandled unknown x,x
tropium nothandled unknown x,x
uridinal nothandled unknown x,x
ustilan nothandled unknown x,x
uval nothandled unknown x,x
uvon nothandled unknown x,x
vanillone nothandled unknown x,x
vinformide nothandled unknown x,x
vulvan nothandled unknown x,x
xanthinol nothandled unknown x,x
zded nothandled unknown x,x
zolamine nothandled unknown x,x
zoxazolamine root root NC2=NC1=CC(C1)=CC=C1O2,x
trans unknown unknown x,x
alltrans unknown unknown x,x
cis unknown unknown x,x
allcis unknown unknown x,x
syn|anti unknown unknown x,x
endo unknown unknown x,x
high unknown unknown x,x
analysis|analytical unknown unknown x,x
aqueous|nonaqueous unknown unknown x,x
laser unknown unknown x,x
phosphoruspentoxide unknown unknown x,x
%|mol|mgml|microgm|glt|mesh|mm|cm|ml|ppm|micron|microns stopword percent x,x
0m|1m|2m|3m|4m|5m|6m|7m|8m|9m|0n|1n|2n|3n|4n|5n|6n|7n|8n|9n stopword percent x,x
ing|ed stopword ing x,x
grade|purity|solution|standardsolution stopword grade x,x
7ci|8ci|9ci|10ci stopword toend x,x
aas|absolute|acn|acs|acsreagent|activator|aerosol|amorphous|analytical stopword
toend x,x
analyzer|anhydrous|approx|assay|atomic stopword toend x,x
balance|beads|bifunctional|biochemical|briquette|briquettes stopword toend x,x
capacity|chelometric|chemiluminescence|certified|chip|chips stopword toend x,x
chiral|chunk|chunks|coarse|colloidal|colorless|concentrate|contains stopword
toend x,x
crucible|crucibles|crude|crystal|crystallites|crystals|crystalline|cube stopword
toend x,x
denatured|determination|dispersion|dry|dust stopword toend x,x

each|electrolytic|electronic|electrophoresis|environmental|esterification|extrac
 tion|extrapure stopword toend x,x
 fcc|filings|fine|finest|flake|flakes|fluorescent|fluorimetric|foil|for|freeradic
 al|from|fume stopword toend x,x
 gas|gauze|gcstandard|glacial|granular|granulate|granule|granules stopword toend
 x,x
 heavy|hplc|hydrophobic stopword toend x,x
 indicator|ingot|ingots|iupac stopword toend x,x
 light|liquid|loose|low|lump|lumps stopword toend x,x
 mainly|maycontain|metal|metals|minimum|moist|mossy stopword toend x,x
 native|natural|needle|needles|notstabilized stopword toend x,x
 on|onactivatedcarbon|optical|organic stopword toend x,x
 particle|pearl|pearls|pellet|pellets|photopolymerization|piece|pieces|plasticize
 r stopword toend x,x
 plate|plates|porous|powder|pract|practical|predominantly|predominatly|primarysta
 ndard|puratronic|pure|purum stopword toend x,x
 reagent|reagentfor|reagentacs|redox|reference|remainder|research|ribbon|ribbons|
 rod|rods stopword toend x,x
 scale|scales|scoop|secondarystandard|selective|sensitive|shaving|shavings|shot
 stopword toend x,x
 simultaneous|singlecrystal|slug|slugs|soft|solid|solution|soot|spectrographic|sp
 ectrophotometric stopword toend x,x
 sphere|spheres|spin|sponge|spray|stab|stabilized|stable|standard|stick|sticks|su
 spension|synthetic|syrup|syrupy stopword toend x,x
 tablet|tablets|tech|technical|thinfoil|titrant|topical|turnings|typically
 stopword toend x,x
 ultra|ultrapure|unstabilized|ultrathinfoil|usp|uvgrade stopword toend x,x
 vial|volumetricstandard stopword toend x,x
 wet|wire|wires|wool stopword toend x,x
 zonerefined stopword toend x,x
 24d|245t|24dnp buildable unknown x,x
 thinfoil|ultrathinfoil|singlecrystal buildable unknown x,x
 antibovine|anticat|antichicken|antidog|antigoat|antiguineapig|antihorse|antihuma
 n|antimonkey|antirabbit|artirat|antisheep notthisversion macromolecule x,x
 tetrahydroprogesterone|tetrahydroprogesteron buildable unknown x,x
 hydrofluoride|hydrochloride|methochloride|methobromide|hydrobromide|hydroiodide|
 hydriodide|methoioidide|methiodide|ethoioidide|ethiodide buildable unknown x,x
 cyclopentadefphenanthren|cyclopentadefphenanthrene buildable unknown x,x
 1011dihydrocinchon|1011dihydrocinchonine|1011dihydrocinchonin|1011dihydroquinidi
 ne|1011dihydrocinchonidine|1011dihydrocinchonidin buildable unknown x,x
 1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
 ydroquinin buildable unknown x,x
 alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin buildable
 unknown x,x
 betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
 bergocryptin|bergocriptine|bergocriptin buildable unknown x,x
 alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin
 buildable unknown x,x
 betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
 riptinine|bergocryptinin|bergocriptinine|bergocriptinin buildable unknown x,x
 1alphah5alphanthropian buildable unknown x,x
 ethylvanillin|ethylcitral buildable unknown x,x
 orthocatechol buildable unknown x,x
 isatoicanhydride buildable unknown x,x
 cresylicacid buildable unknown x,x
 chlorosulfamicacid buildable unknown x,x

hexafluorophosphoricacid|hexafluorosilicicacid|hexafluorozirconicacid|tetrafluoroboricacid buildable unknown x,x
ylcation|ylanion buildable unknown x,x
betaalan buildable unknown x,x
crotonylalcohol buildable unknown x,x
betainealdehyde|betainaldehyd buildable unknown x,x
biotinamide|biotinamid buildable unknown x,x
angeldust buildable unknown x,x
catecholborane buildable unknown x,x
vitaminb1nitrate|thiaminenitrate|thiaminnitrate|thiaminechloride|thiaminchlorid buildable unknown x,x
44'carbocyanine|22'carbocyanine buildable unknown x,x
ylthiol buildable unknown x,x
benzeneoxid|benzeneoxide buildable unknown x,x
card|2022cardenolide|card2022enolide buildable unknown x,x
25norbornadien|25norbornadiene|2norbornene|2norbornen|5norbornene|5norbornen buildable unknown x,x
icalcohol buildable unknown x,x
orthophthal buildable unknown x,x
neopentylglycol buildable unknown x,x
nitrogendioxide|nitricoxide|nitrousoxide buildable unknown x,x
hydrogenphosphato|dihydrogenphosphato buildable unknown x,x
chloralhydrate|bromalhydrate buildable unknown x,x
vinylsulfurol buildable unknown x,x
arsenicacid buildable unknown x,x
methacr buildable unknown x,x
formamidinedisulfide buildable unknown x,x
isonitroso|isonitros|isonipecot|isobenzofuran|isocrotono|isocroton|isocrot|isoquinol|isochinol|glutathionereduced buildable unknown x,x
3thiotriphosphor|2thiodiphosphor buildable unknown x,x
alphalinolen|gammalinolen buildable unknown x,x
alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalphaglycerophosph buildable unknown x,x
alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dlalphaglycerophospho buildable unknown x,x
betaoestradiol|betaestradiol buildable unknown x,x
dicarboxylicimide|dicarboxylicacidimide buildable unknown x,x
hydrogentartrate|hydrogenltartrate|hydrogendtartrate|lbitartrate|dbitartrate|hydrogenmaleate|hydrogenoxalate|hydrogensulfate|hydrogensulfite|hydrogensulfide buildable unknown x,x
alphaionon|alphaionone|betaionone|betaionon buildable unknown x,x
sulfurdiimide|sulfurdiimid buildable unknown x,x
snglycerol|snglycero|racglycerol|racglycero buildable unknown x,x
orthophosphor buildable unknown x,x
uvgrade buildable unknown x,x
ionchromatography buildable unknown x,x
dewarbenzene buildable unknown x,x
alloisoleuc|allothreono|allothreon buildable unknown x,x
anaphthoflavone|alphanaphthoflavone|bnaphthoflavone|betanaphthoflavone buildable unknown x,x
gcstandard|primarystandard|secondarystandard buildable unknown x,x
purineriboside buildable unknown x,x
secpheneth buildable unknown x,x
4nitroanilide|pnitroanilide buildable unknown x,x
betacitronell buildable unknown x,x
methylviologen|ethylviologen|benzylviologen buildable unknown x,x
zirconyliv|vanadyliv buildable unknown x,x

activatedcarbon|onactivatedcarbon buildable unknown x,x
 extrapure buildable unknown x,x
 maycontain buildable unknown x,x
 volumetricstandard buildable unknown x,x
 notstabilized buildable unknown x,x
 zonerefined buildable unknown x,x
 standardsolution buildable unknown x,x
 wt buildable unknown x,x
 phosphorustriamide buildable unknown x,x
 nepsilon buildable unknown x,x
 betacarboline buildable unknown x,x
 pentamethylenetetramine|pentamethylenetetramin buildable unknown x,x
 hexamethylenetetramine|hexamethylenetetramin buildable unknown x,x
 ochloranil|mchloranil|pchloranil buildable unknown x,x
 mesoinositol|myoinositol|dinositol|linositol|scylloinositol|epiinositol
 buildable unknown x,x
 stainlesssteel buildable unknown x,x
 alphafuril buildable unknown x,x
 alphapinene|betapinene buildable unknown x,x
 chrysoidiner buildable unknown x,x
 naphtholas buildable unknown x,x
 neutralbuffer buildable unknown x,x
 alphacumyl buildable unknown x,x
 alphaphellandrene|betaphellandrene buildable unknown x,x
 bisphenola buildable unknown x,x
 alphasorcy|alip buildable unknown x,x
 alphasorcy|aresorcy|betaresorcy|bresorcy|gammaresorcy|gresorcy buildable
 unknown x,x
 gerani buildable unknown x,x
 lascorb buildable unknown x,x
 vitaminh|vitaminb1|thiaminedisulfide|vitaminb2|vitamine|alphatocopherol|atocophe
 rol buildable unknown x,x
 vitamind3 buildable unknown x,x
 phenolsulfonphthalein|phenolsulfonephthalein|mresolsulfonphthalein|mresolsulfo
 nephthalein|ocresolsulfonphthalein|ocresolsulfonephthalein|pyrocatecholsulfonpht
 halein|pyrocatecholsulfonephthalein|pyrogallolsulfonphthalein|pyrogallolsulfonep
 hthalein|thymolsulfonphthalein|thymolsulfonephthalein|phenolphthalein|mresolpht
 halein|ocresolphtalein|pyrocatecholphtalein|pyrogallolphtalein|thymolphtalei
 n buildable unknown x,x
 freeradical buildable unknown x,x
 obenzeno buildable unknown x,x
 ptoluquinone|pxyloquinone buildable unknown x,x
 cyclopentaaphenanthrene|cyclopentaaphenanthren buildable unknown x,x
 pdioxine|mdioxine|pdioxin|mdioxin buildable unknown x,x
 asindacene|asindacen|sindacene|sindacen buildable unknown x,x
 sendachromeal buildable unknown x,x
 isonicotino|isonicotin buildable unknown x,x
 leucicacid buildable unknown x,x
 isoser buildable unknown x,x
 isoval buildable unknown x,x
 isoleuc buildable unknown x,x
 tleuc|tertleuc buildable unknown x,x
 orthotyros buildable unknown x,x
 mtyros|metatyros buildable unknown x,x
 ptyros|paratyros buildable unknown x,x
 hydroxyprol|3hydroxyprol|4hydroxyprol|5hydroxyprol buildable unknown x,x
 3phenylalan|betaphenylalan buildable unknown x,x

dtartar|dtartr|mesotartar|mesotartr buildable unknown x,x
 tetrafluoroborate|tetrafluoroboratel buildable unknown x,x
 fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat buildable
 unknown x,x
 onnazoxy|nnoazoxy|nonazoxy buildable unknown x,x
 glycolacetal|glycolketal buildable unknown x,x
 moll|mgml|microgml|glt|reagentfor|reagentacs|acsreagent buildable unknown x,x
 ptosylate|ptosyl buildable unknown x,x
 oxazine1|oxazine4 buildable unknown x,x
 tboc buildable unknown x,x
 iumion|ideion|iuncation|ideanion buildable unknown x,x
 isobutyro|isobutyr buildable unknown x,x
 isovalero|isovaler buildable unknown x,x
 isophthalo|mpthalo|isophthal|mpthal buildable unknown x,x
 terephthalo|ppthalo|terephthal|ppthal buildable unknown x,x
 etherof buildable unknown x,x
 esterswith|estersof|esterwith|esterof buildable unknown x,x
 saltof buildable unknown x,x
 iclactone|iclacton buildable unknown x,x
 iclactam buildable unknown x,x
 anhydridewith buildable unknown x,x
 cyclicanhydride buildable unknown x,x
 phosphoruspentoxide buildable unknown x,x
 allcis buildable unknown x,x
 alltrans buildable unknown x,x
 acinitro buildable unknown x,x
 astriazine|astriazin|striazine|striazin|asymtriazine|asymtriazin|symtriazine|sym
 triazin buildable unknown x,x
 astrioxane|astrioxan|strioxane|strioxan|asymtrioxane|asymtrioxan|symtrioxane|sym
 trioxan buildable unknown x,x
 astriazino|striazino|asymtriazino|symtriazino buildable unknown x,x
 astrioxano|strioxano|asymtrioxano|symtrioxano buildable unknown x,x
 astrithiane|astrithian|strithiane|strithian|asymtrithiane|asymtrithian|symtrithi
 ane|symtrithian buildable unknown x,x
 thiurammonosulfide|thiuramdisulfide|thiuramtrisulfide|thiuramtrisulfid|thiuramte
 trasulfide|thiuramtetrasulfid buildable unknown x,x
 isourea|isothiourea|lisoureido|3isoureido|1isothioureido|3isothioureido|1isosele
 noureido|3isoselenoureido|1isotelluroureido|3isotelluroureido buildable unknown
 x,x
 ' typo typo '
 " typo typo ''
 ± typo typo +/-
 μ typo typo mu
 , - typo typo -
 § typo typo beta
 -> typo typo -fwdarw-
 (alpha) typo typo alpha
 (beta) typo typo beta
 (gamma) typo typo gamma
 (delta) typo typo delta
 (epsilon) typo typo epsilon
 (omega) typo typo omega
 (ortho) typo typo ortho
 (meta) typo typo meta
 (para) typo typo para
 (tau) typo typo tau
 -oxyl typo typo -oxylradical

-thiolate typo typo -mercaptide
 1-dimethylaminonaphthalene-5-sulfonyl typo typo dansyl
 1,2-o-isopropylidene-d-glycer typo typo 2,3-o-isopropylidene-d-glycer
 1,2-o-isopropylidene-1-glycer typo typo 2,3-o-isopropylidene-1-glycer
 1,2-o-isopropylidene-glycer typo typo 2,3-o-isopropylidene-glycer
 1alphah,5alphah typo typo 1alphah5alphah
 a.c.s typo typo acs
 acetamin typo typo acetonylamin
 acxid typo typo acid
 adonitol typo typo ribitol
 aicd typo typo acid
 aldazine typo typo aldehydeazine
 all-e typo typo all-cis
 all-z typo typo all-trans
 allose typo typo alloose
 allofuranose typo typo alloofuranose
 allopyranose typo typo alloopyranose
 alpha-tolual typo typo phenylacetal
 alpha-toluat typo typo phenylacetat
 alpha-toluic typo typo phenylacetic
 alpha-tolunitril typo typo phenylacetoneitril
 aluminium typo typo aluminum
 amidosulfon typo typo amidosulfur
 amimo typo typo amino
 ammin typo typo amin
 anonan typo typo a-nonan
 anonyl typo typo a-nonyl
 azodicarbonamide typo typo azodicarboxamide
 bathophenanthroline typo typo bathophenanthroline
 benez typo typo benz
 benzamin typo typo benzenamin
 benzhydrazid typo typo benz-hydrazid
 benzhydroxam typo typo benz-hydroxam
 benzotriazol typo typo benzotriazolyl
 bisoleam typo typo bis-oleam
 bismeth typo typo dimeth
 borinan typo typo bor-inan
 caes typo typo ces
 capro typo typo hexano
 caprin typo typo decan
 carboselen typo typo carboxselen
 carbotellur typo typo carboxtellur
 carbothi typo typo carboxthi
 carboxamide typo typo carboxylamide
 chinone typo typo quinone
 chlorobromide typo typo chloridebromide
 chlorofluoride typo typo chloridefluoride
 chloroformate typo typo (chloroformate)
 cinnamid typo typo cinnamamid
 cis/trans typo typo cis+trans
 collidin typo typo trimethylpyridin
 columb typo typo niob
 crotonitrile typo typo crotononitrile
 dextrose typo typo d-glucose
 dicaprin typo typo dicapr-in
 diethylenetriaminepenta typo typo diethylenetriamine-n,n,n',n',n''-penta
 diethylenetriamine-penta typo typo diethylenetriamine-n,n,n',n',n''-penta

diolate type type di-olate
dioleoyl type type di-oleoyl
dionate type type -dionate
diphosphate type type diphosphate
ehty type type ethy
endo, type type endo-
erythrul type type glycerotetrul
ethinyl type type ethynyl
ethylenebis type type ethylene-bis-
ethylenediaminetetra type type ethylenediamine-n,n,n',n'-tetra
ethylhexoxid type type ethylhexanoxid
etyl type type ethyl
exo, type type exo-
flour type type fluor
fluoronon type type fluoro-non
fluoro type type fluoro
furanuron type type furanoseuron
fruct type type arabinohexul
fucosyl type type fucoseyl
galactosyl type type galactoseyl
gamma-collidin type type 2,4,6-trimethylpyridin
glucosyl type type glucoseyl
glucuronide type type glucosiduronicacid
guanad type type guanid
hydrofluoren type type hydro-fluoren
idose type type idoose
idofuranose type type idoofuranose
idopyranose type type idoopyranose
imadaz type type imidaz
imdaz type type imidaz
inosinate type type inosate
inosinic type type inosic
iso- type type iso
levulo type type arabinohexulo
linalyl type type linaloyl
lupetid type type dimethylpiperid
lutid type type dimethylpyrid
mol/l type type moll
monocaprin type type monocapr-in
mononitrile type type mono-nitrile
monoole type type mono-ole
mucic type type galactaric
n'n' type type n',n'
n-alpha type type nalpha
n-(alpha) type type nalpha
n-gamma type type ngamma
n-delta type type ndelta
n-omega type type nomega
n-im- type type nim
naphta type type naphtha
naphthaldehyde type type naphthaldehyde
naphthalic type type naphthalenedicarboxylic
naphthalimid type type naphthalenedicarboximid
naphty type type naphthy
naphthyrid type type diazanaphthalene
napta type type naphtha
naph type type naphth

napyty typo typo naphthy
 ocineol typo typo o-cineol
 oxamide typo typo oxalicamide
 oxeturon typo typo oxetoseuron
 oxiruron typo typo oxiroseuron
 oxylenol typo typo o-xyleneol
 p-naphthoquinone typo typo 1,4-naphthoquinone
 pentacyclohexylammonium typo typo penta(cyclohexylammonium)
 peracet typo typo peroxyacet
 phath typo typo phth
 phenanthroline typo typo diazabenz[a]naphthalene
 phosphonyl typo typo phosphonoyl
 phosphorin typo typo -phosphorin
 phosphoryl typo typo phosphoroyl
 phthal typo typo phthal
 phthaldehyde typo typo phthalaldehyde
 proprion typo typo propion
 pthal typo typo phthal
 psico typo typo ribohexulo
 pyranuron typo typo pyranoseuron
 rhodate typo typo rhodaate
 ribul typo typo erythropentul
 rosinat typo typo abietate
 s-triazol typo typo 1,2,4-triazol
 sacchar typo typo glucar
 saccharin typo typo saccharin
 saccharid typo typo saccharid
 salycyl typo typo salicyl
 selenious typo typo selenous
 septanuron typo typo septanuron
 siloxid typo typo silanoxid
 sorbo typo typo xylohexulc
 sorbitol typo typo glucitol
 stilbazol typo typo styrylpyridin
 sufo typo typo sulfo
 sulfamidic typo typo sulfamic
 sulfamyl typo typo sulfamoyl
 sulfohydrazide typo typo sulfonohydrazide
 sulph typo typo sulf
 sulphamyl typo typo sulfamoyl
 sulphohydrazide typo typo sulfonohydrazide
 tagat typo typo lyxohexul
 tetracarboxdiimide typo typo bis(dicarboximide)
 tetrahydridoborato typo typo tetrahydridoborate
 tetrphosphate typo typo tetraphosphorate
 thiazyl typo typo thiazolyl
 thiocarbamyl typo typo thiocarbamoyl
 thiol- typo typo thiole-
 thiolan typo typo thi-olan
 thiolylium typo typo thiole-ylium
 thionochloroform typo typo chlorothionoform
 thiooxine typo typo thio(oxine)
 thiophen- typo typo thiophene-
 thiophenamine typo typo thiophene-amine
 thiophenic typo typo thiopheneic
 thiophenone typo typo thiophene-one
 threonate typo typo threonate

threonic typo typo threonic
 tricaprin typo typo tricapr-in
 tricaproin typo typo trihexanoin
 trichloromethylsulfen|trichloromethanesulfen typo typo (trichloromethyl)sulfen
 trifluoromethylsulfen|trifluoromethanesulfen typo typo (trifluoromethyl)sulfen
 trioleate typo typo (tris)oleate
 triolein typo typo tri-ole-in
 trioleoyl typo typo (tris)oleoyl
 trioleyl typo typo (tris)oleyl
 triphosphate typo typo triphosphate
 trithioperoxy typo typo thiodithioperoxy
 tritolyl typo typo tristolyl
 tropilidene typo typo 2,4,6-cyclohexatriene
 tyrosinate typo typo tyrosin-ate
 uloson typo typo ulo-on
 xanthylic typo typo xanthonylic
 xylul typo typo threopentul
 acidic notthisversion unknown x,x
 activatedcarbon notthisversion bulksolid x,x
 agarose notthisversion macromolecule x,x
 agar notthisversion macromolecule x,x
 agglutinin notthisversion macromolecule x,x
 albumin notthisversion macromolecule x,x
 alkonium notthisversion mixture x,x
 alkyl|alkyl* notthisversion mixture x,x
 alloy notthisversion bulksolid x,x
 algin notthisversion macromolecule x,x
 alumina notthisversion bulksolid x,x
 amalgam notthisversion bulksolid x,x
 amyloid notthisversion macromolecule x,x
 amylose notthisversion macromolecule x,x
 angiotensin notthisversion macromolecule x,x
 anthocyanidin notthisversion mixture x,x
 anthocyanin notthisversion mixture x,x
 antibody notthisversion macromolecule x,x
 antibovine notthisversion macromolecule x,x
 anticat notthisversion macromolecule x,x
 antichicken notthisversion macromolecule x,x
 antidog notthisversion macromolecule x,x
 antigoat notthisversion macromolecule x,x
 antiguineapig notthisversion macromolecule x,x
 antihorse notthisversion macromolecule x,x
 antihuman notthisversion macromolecule x,x
 antimonkey notthisversion macromolecule x,x
 antirabbit notthisversion macromolecule x,x
 antirat notthisversion macromolecule x,x
 antisheep notthisversion macromolecule x,x
 ase notthisversion macromolecule x,x
 asphalt notthisversion mixture x,x
 avidin notthisversion macromolecule x,x
 azure notthisversion color x,x
 bacitracin notthisversion macromolecule x,x
 bead|beads notthisversion bulksolid x,x
 bentonite notthisversion bulksolid x,x
 black notthisversion color x,x
 block notthisversion polymer x,x
 blue notthisversion color x,x

bombesin notthisversion macromolecule x,x
 bradykinin notthisversion macromolecule x,x
 brij notthisversion polymer x,x
 brilliant notthisversion color x,x
 bromelian notthisversion macromolecule x,x
 broth notthisversion mixture x,x
 brown notthisversion color x,x
 buckyball|buckyballs notthisversion fullerene x,x
 buffer notthisversion mixture x,x
 calcia notthisversion bulksolid x,x
 calcitonin notthisversion macromolecule x,x
 carborundum notthisversion bulksolid x,x
 carmine notthisversion color x,x
 carrageenan notthisversion macromolecule x,x
 casein notthisversion macromolecule x,x
 casomorphin notthisversion macromolecule x,x
 celite notthisversion bulksolid x,x
 cells notthisversion bulksolid x,x
 cellulose notthisversion macromolecule x,x
 cephalin|cephalins notthisversion mixture x,x
 ceria notthisversion bulksolid x,x
 charcoal notthisversion bulksolid x,x
 chelate notthisversion mixture x,x
 chitin notthisversion macromolecule x,x
 chitosan notthisversion macromolecule x,x
 cholecystokinin notthisversion macromolecule x,x
 chondroitin notthisversion macromolecule x,x
 cocktail notthisversion mixture x,x
 coco notthisversion mixture x,x
 collagen notthisversion macromolecule x,x
 collodion notthisversion macromolecule x,x
 concanavalin notthisversion macromolecule x,x
 conotoxin notthisversion macromolecule x,x
 demi notthisversion hemi x,x
 detergent|detergent notthisversion mixture x,x
 dextrin|dextran notthisversion macromolecule x,x
 dna notthisversion macromolecule x,x
 dowex notthisversion polymer x,x
 drierite notthisversion bulksolid x,x
 dynorphin notthisversion macromolecule x,x
 edestin notthisversion macromolecule x,x
 endorphin notthisversion macromolecule x,x
 endothelin notthisversion macromolecule x,x
 enzyme|enzymes notthisversion macromolecule x,x
 emulsin notthisversion macromolecule x,x
 extract notthisversion mixture x,x
 fatty notthisversion mixture x,x
 ferritin notthisversion macromolecule x,x
 fibrin notthisversion macromolecule x,x
 fibrinogen notthisversion macromolecule x,x
 fibrinolysin notthisversion macromolecule x,x
 fibronectin notthisversion macromolecule x,x
 ficin notthisversion macromolecule x,x
 ferrocene|ferrocen notthisversion inorgcomplex x,x
 flavor notthisversion mixture x,x
 fraction notthisversion mixture x,x
 fullerene|fullerenes notthisversion fullerene x,x

galactan notthisversion polymer x,x
 gelatin|gelatine notthisversion macromolecule x,x
 gliadin notthisversion macromolecule x,x
 globulin notthisversion macromolecule x,x
 glove|gloves notthisversion bulksolid x,x
 gluten notthisversion macromolecule x,x
 glutenin notthisversion macromolecule x,x
 gonadotropin notthisversion macromolecule x,x
 graphite notthisversion bulksolid x,x
 green notthisversion color x,x
 grey|gray notthisversion color x,x
 gum notthisversion mixture x,x
 hemi notthisversion hemi x,x
 hemoglobin notthisversion macromolecule x,x
 heparin|heparan notthisversion macromolecule x,x
 histone notthisversion macromolecule x,x
 hormone notthisversion macromolecule x,x
 hyaluron notthisversion macromolecule x,x
 hydrocarbon|hydrocarbons notthisversion mixture x,x
 insulin notthisversion macromolecule x,x
 interferon notthisversion macromolecule x,x
 interleukin notthisversion macromolecule x,x
 inulin notthisversion macromolecule x,x
 isotope notthisversion isotope x,x
 kaolin notthisversion macromolecule x,x
 kephalin notthisversion macromolecule x,x
 keratin notthisversion macromolecule x,x
 kerosene|kerosine notthisversion mixture x,x
 kit notthisversion mixture x,x
 kitasamycin notthisversion mixture x,x
 lake notthisversion color x,x
 laminaran notthisversion macromolecule x,x
 lanolin notthisversion macromolecule x,x
 latex notthisversion polymer x,x
 lecithin notthisversion macromolecule x,x
 lectin notthisversion macromolecule x,x
 lignine|lignin notthisversion macromolecule x,x
 ligroin|ligroine notthisversion mixture x,x
 litmus notthisversion macromolecule x,x
 lysozyme notthisversion macromolecule x,x
 magenta notthisversion color x,x
 mannan notthisversion macromolecule x,x
 mixed|mixt|mixture|mixtures notthisversion mixture x,x
 mer|mers notthisversion polymer x,x
 merase notthisversion macromolecule x,x
 mu notthisversion inorgcomplex x,x
 mucin notthisversion macromolecule x,x
 myoglobin notthisversion macromolecule x,x
 myosin notthisversion macromolecule x,x
 naphthen notthisversion macromolecule x,x
 neurokinin notthisversion macromolecule x,x
 neurotensin notthisversion macromolecule x,x
 nigrosine notthisversion macromolecule x,x
 norit notthisversion bulksolid x,x
 nucle notthisversion macromolecule x,x
 nuclein notthisversion macromolecule x,x
 nylon notthisversion polymer x,x

ocene|ocen notthisversion inorgcomplex x,x
oil notthisversion mixture x,x
orange notthisversion color x,x
pancreatin notthisversion macromolecule x,x
papain notthisversion macromolecule x,x
paraffin notthisversion bulksolid x,x
paraformaldehyde notthisversion polymer x,x
parathyroid notthisversion macromolecule x,x
pectin notthisversion macromolecule x,x
pepsin notthisversion macromolecule x,x
peptide notthisversion macromolecule x,x
peptone notthisversion macromolecule x,x
petrol|petroleum notthisversion mixture x,x
pink notthisversion color x,x
pipe notthisversion bulksolid x,x
pollen notthisversion bulksolid x,x
poly|polymer|polymers|homopolymer notthisversion polymer x,x
protamine notthisversion macromolecule x,x
protein notthisversion macromolecule x,x
pullulan notthisversion macromolecule x,x
purple notthisversion color x,x
quinhydrone notthisversion mixture x,x
red notthisversion color x,x
rennin notthisversion macromolecule x,x
resin notthisversion polymer x,x
rna notthisversion macromolecule x,x
salmine notthisversion macromolecule x,x
sand notthisversion bulksolid x,x
saponin notthisversion macromolecule x,x
scarlet notthisversion color x,x
semi notthisversion hemi x,x
serum notthisversion macromolecule x,x
sesqui notthisversion hemi x,x
sieve|sieves notthisversion bulksolid x,x
silica|silicagel notthisversion bulksolid x,x
somatostatin notthisversion macromolecule x,x
somatotropin notthisversion macromolecule x,x
stainlesssteel notthisversion bulksolid x,x
starch notthisversion macromolecule x,x
streptavidin notthisversion macromolecule x,x
streptomycin notthisversion macromolecule x,x
strip|strips notthisversion bulksolid x,x
talc notthisversion bulksolid x,x
tallow notthisversion mixture x,x
tann notthisversion macromolecule x,x
thaumatin notthisversion macromolecule x,x
thoria notthisversion bulksolid x,x
thrombin notthisversion macromolecule x,x
titania notthisversion bulksolid x,x
tragacanth notthisversion macromolecule x,x
transferrin notthisversion macromolecule x,x
triton notthisversion polymer x,x
trypsin notthisversion macromolecule x,x
tube|tubes notthisversion bulksolid x,x
tween notthisversion polymer x,x
tylose notthisversion macromolecule x,x
valve notthisversion bulksolid x,x

vasopressin notthisversion macromolecule x,x
 venom notthisversion mixture x,x
 violet notthisversion color x,x
 wax notthisversion bulksolid x,x
 white notthisversion color x,x
 xylan notthisversion macromolecule x,x
 yeast notthisversion bulksolid x,x
 yellow notthisversion color x,x
 yttria notthisversion bulksolid x,x
 zein notthisversion macromolecule x,x
 zeolite notthisversion bulksolid x,x
 zephiran notthisversion macromolecule x,x
 zephirol notthisversion macromolecule x,x
 zirconia notthisversion bulksolid x,x
 zyme notthisversion macromolecule x,x
 ortho ordinal ordinal x,x
 epsilon ordinal ordinal x,x
 nepsilon ordinal ordinal x,x
 npi ordinal ordinal x,x